Group Representation Theory for Physicists

2nd Edition

Jin-Quan Chen, Jialun Ping & Fan Wang

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GROUP REPRESENTATION THEORY FOR PHYSICISTS, 2nd Edition

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Foreword to the first edition

A new generation of books on group theory for physicists has appeared over the last ten years. Many of them deal only with elementary particle physics or with condensed matter physics. This volume by Prof. Jin–Quan Chen is a serious attempt to cover a broad range of applications of group theory to physics. It begins with an introduction to the elements of group theory and the theory of representations. Representations of finite groups and character theory are carefully treated and applied in later chapters to point groups and space groups, where thorough and practical information is given about molecular and crystal groups.

The permutation group is discussed in detail, and its use in finding the irreducible representations of unitary groups is carefully and completely covered. Lie groups and Lie algebras are treated sufficiently to enable their use in elementary particle physics, with a thorough presentation of Dynkin diagrams and the reduction of products.

For spectroscopy and, in particular, nuclear spectroscopy, this is the first up–to–date and thorough treatment of the calculation of isoscalar factors and coefficients of fractional parentage. There are extensive tables and indications of computational methods.

With his collaborators in Nanjing and Philadelphia, Chen has contributed extensively to new developments over the past decade. These researches are incorporated into the present book, of which a preliminary version was published a few years ago in the People's Republic of China.

It has been a pleasure for me to talk with Chen many times about group theory and a special pleasure to welcome the appearance of this book.

Morton Hamermesh
University of Minnesota

Preface to the first edition

Conscious of the frustration we experienced as we tried to learn group theory, and apply it to problems in physics, Fan Wang, Mei Juan Gao and I endeavored in 1974 to carry out a systematic reform of standard, or traditional group representation theory. Our aim was to establish a new approach to group representations in accordance with the concept and method used in quantum mechanics, so that it would be much more accessible to physicists and chemists.

The breakthrough came in late 1974. A new approach to group representation gradually came into being and with it a new method, the eigenfunction method (EFM), emerged for finding primitive characters, irreducible bases, Clebsch–Gordan (CG) coefficients, etc. From 1976–1978, the EFM was translated into codes and for the first time the CG coefficients and the outer–product reduction coefficients for the permutation group S_2–S_6 were computed by the EFM. The EFM was extended in 1979 to the computation of the CG coefficients, Racah coefficients, isoscalar factors, subduction coefficients of unitary groups. From 1981–1987, the new approach was applied to space groups and graded unitary groups and established several codes for space groups, SU(n) CG coefficients, SU(mn) $\supset$ SU(m) $\times$ SU(n) and SU($m+n$) $\supset$ SU(m)$\times$ SU(n) coefficients of fractional parentage, and so on.

The new approach has been introduced at various universities and institutions, such as the City College of the City University of New York, the University of Chicago, Clarkson, Dalhousie, Drexel, Duke, Hong Kong, Minnesota, Maryland, Montreal, Singapore, Yale, and Los Alamos National Laboratory, as well as at the IXth and XIVth International Colloquium on Group Theoretical Method in Physics held in Mexico 1980, and Seoul 1985, respectively.

The Chinese book *A New Approach to Group Representation Theory* was written in 1981 and published in 1985 and has since been used as a textbook in Nanjing University for undergraduate and graduate students. Prior to the publication of the Chinese book, the manuscript had been used as a textbook in Nanjing University and Drexel University in Philadelphia.

The present book was based on the Chinese book and the new developments during the period of 1981–1987. All chapters except chapters 4 and 7 have been re–written.

I am indebted to my collaborators Mei–Juan Gao who took part in the writing of Chapter 8 and performed most of the practical computations, Guang–Qun Ma who was involved in the writing of Chapter 10, and it is he who first attempted to use the EFM to treat the space group representation, Fan Wang and Xuan–Gen Chen for their invaluable suggestions and criticism. I am grateful to Professors Xiao–Qian Zhou, Shi–Shu Wu and Duan Feng for their constant encouragement and patient reading of the manuscript. Thanks are due also to Professors Tan Lu, Fu–Cho Pu, Qin–Yue Qu, Hong–Zhou Sun, Rui–Bao Tao, Cheng–Li Wu, Rong–Jue Wei, Xi–De Xie and Guang–Xiang Xu for their enthusiasm in this work and support. I am grateful to many students who have offered helpful criticism and raised challenging questions.

Mr. Pei–Ning Wang typed the initial draft of Chapters 4–9, and my son, Bing–Qing wrote several software codes for facilitating the typing and proof–reading of the manuscript. Without their help it would be inconceivable that the re–writing could have been accomplished within

half a year.

Special mention must be made of Professors B. Bayman, M. Hamermesh and K.T. Hecht for their constant interest and many illuminating discussions, and D.H. Feng, who gave me the opportunity and encouragement to teach a course on group theory at Drexel University.

Last but not least I would like to thank Professors L. C. Biedenharn, J. Birman, U. Fano, R. Gilmore, J. Ginocchio, J. J. Griffin, F. Iachello, J. Paldus, J. Patera and K. K. Phua for their stimulating discussions and the hospitality extended to me during my visits to their institutions.

Nanjing University Jin-Quan Chen
March, 1987

Preface to the second edition

Ten years have passed since the publication of the first edition of this book in which a complete set of commuting operators (CSCO) approach to the group representation theory was proposed. During this period, several remarkable advances of relevance have been made. A common feature of these new developments is that they give algebraic expressions for some useful coefficients of the following groups:

1. Quantum groups $U_q(n)$ (Pan & Chen 1993).

2. Orthogonal groups O_n and symplectic groups $Sp(2n)$ (Pan & Dai, 1996, Pan, Dong & Draayer, 1997, 1998).

3. Unitary groups and permutation groups with irreducible representations involving two columns (Li & Paldus, 1990, 1993).

4. Point groups (Chen & Fan 1998, Fan & Chen, 1999, Fan, Chen & Draayer 1999).

The first three will not be covered in this book but will be mentioned in appropriate places in the book, while some new results for point groups will be introduced in Chapter 8.

In the 1989 edition of the book, the projection operator method, the most commonly used method in standard textbooks on group theory, was essentially ignored. We mentioned only the main steps and discussed its serious shortcomings. Instead we developed the eigenfunction method (EFM) and urged its use. Ten years later, the wheel has gone full circle, and it is time to re–assess the power of the projection operator method. With the discovery of algebraic expressions for the projection operators, the projection operator method becomes extremely simple and powerful for point groups. An interesting point though is that only with the help of the EFM are these algebraic expressions obtainable. So we have a good example of negating a negation. The projection operator returns, albeit in a new form.

In this edition the following sections are new:

Sec. 3.14. Irreducible basis vectors in non–orthogonal reducible basis.

Sec. 5.9. The groups U_{2j+1}, SO_{2l+1} and Sp_{2j+1}.

Sec. 7.20. The generalized quantized expressions for the coefficients of fractional parentage.

Sec. 9.8. The Groups Sp_N, SO_N and the pairing interaction.

Sec. 9.2. Nuclear shell model: Multi–shell.

Most parts of Chapter 8 on the point groups have been rewritten. The new contents include a preliminary introduction of the algebraic solutions and a detailed discussion of the double–valued representations of point groups.

The assistance of Dr. L. McAven and Prof. C. W. Wong has been invaluable in preparing this edition, and I am very grateful to them both. Dr. McAven helped with the drawing of all of the figures, checked the text and formulas, and assisted with layout issues. Prof. C. W. Wong carefully read the book, in particular improving upon the exposition of Sec. 3.9.3. Discussions with Drs. Peng–Dong Fan, S. E. Bernades and Hong–Zhou Sun have also been useful.

Nanjing University Jin–Quan Chen
Dec., 1999

Addendum

As mentioned by Prof. J. Q. Chen in the preface of the first edition, we started to reform the group representation theory in accordance with the concept and method of quantum mechanics in 1974. Because both of us kept an idea that due to the group theory was solely developed by mathematicians, so it does not match the quantum physics well and it should be possible to have a group representation theory which matches quantum physics as harmonious as the relation between calculus and the classical physics. Such a reform was realized in 1974-1980. Since 1977 I was interested in the hadron physics based on quantum chromodynamics inspired models and gradually shifted to that field. All the further developments after 1981 were by Chen himself and later with collaboration with Jia-Lun Ping and Feng Pan except the application of the new representation theory in the quark model calculations.

Prof. J. Q. Chen passed away untimely on May 14, 2000. This second edition is almost finished by Chen himself. As a lifelong colleague of Prof. Chen, I am duty-bound to make it published. The unfinished work is mainly done by Prof. Jia-Lun Ping.

We offer this book to the community interested in the application of group theory as a monument of Prof. Chen. It includes every contributions of Prof.Chen to the group theory and its applications except the graded Lie group and quantum group which Prof. Feng Pan will explain it in the memorial volume "The Intellectual Path of J. Q. Chen: A Memorial".

Fan Wang
February, 2002 at Nanjing

Contents

Chapter 5 Lie Groups

Contents of Some Important Tables

Glossary

1. Group

E	Euclidean group
G	a group
$\mathcal{G}$	a representation group
$\overline{G}$	Intrinsic group of G
$\mathbf{G}$	a space group, or an abstract group
$\mathbf{G}^\dagger$	double group or double space group
$\mathbf{g}$	a point group
$\mathbf{G}_0$	isogonal point group of the space group $\mathbf{G}$
$\mathbf{G}_0(\mathbf{k})$	little co–group, (10-57a)
$G(\mathbf{k})$	little group, (10-58)
$\mathbf{G}_\mathbf{k}, \mathbf{G}'_\mathbf{k}$	representation groups, (10-63c), (10-70)
G_s	a subgroup of G
$G(s) = G(1) \supset G(2) \supset \dots$	a canonical subgroup chain of G
$\overline{G}(s) = \overline{G}(1) \supset \overline{G}(2) \supset \dots$	a canonical subgroup chain of $\overline{G}$
$G(s')$	a non–canonical subgroup chain
$\mathbf{P}$	holosymmetric point group of a crystal system, (10-17)
$\mathbf{P}(\mathbf{k})$	symmetric group of $\mathbf{k}$, (10-50)
$S_n(\mathcal{S}_n)$	permutation group in coordinate (state) space
$S_n(\omega)$	a permutation group in the indices (ω)
$\mathbf{T}$	translation group, or lattice group
$U_n, SU_n(\mathcal{U}_n, \mathcal{SU}_n)$	unitary group in coordinate (state) space

2. Group elements

$a, R_a, R(a), R, S, T, \dots$	group elements
α, β, γ	group elements of a point group
p	permutation operator in coordinate space, (3-108)
$\wp$	permutation operator in state space, (3-107)
$Q = \binom{\omega_0}{\omega}$	order–preserving permutation, (4-131)
$R_i = \{\gamma_i \vert \mathbf{V}(\gamma_i)\}'$ $= \exp[i\mathbf{k}\cdot\mathbf{V}(\gamma_i)]\{\gamma_i \vert \mathbf{V}(\gamma_i)\}$	group element of the rep group $G'_\mathbf{k}$, (10-66)

3. Spaces and basis vectors

$L, \mathcal{L}$	any rep space
L_g	group space of a group G, or a rep group G
$L_c(L_n)$	class space of a group G (a rep group $G'_\mathbf{k}$)
L_ν	eigenspace of the CSCO–I of $G, L \subset L_g$
$\mathcal{L}_\nu$	eigenspace of the CSCO–I of $G, \mathcal{L}_\nu \subset \mathcal{L}$
$L_{(\nu)k}$	the k–th irreducible space of G
$L(\mathbf{k})$	group space of the rep group $G'_\mathbf{k}$, (10-73b)
$\mathcal{L}_\mathbf{k}$	eigenspace of translation operator $\{\varepsilon \vert \mathbf{R}_n\}$, (10-54b)
$\mathcal{L}(*\mathbf{k})$	representation space of a space group $\mathbf{G}$, (10-55c)
$\vert\omega_0\rangle = \vert i_1 i_2 \dots i_n\rangle$	normal order state, (3-106)
$\vert\omega\rangle = \vert i_1 i_2 \dots i_n\rangle$	normal order state (with repeated state labels)

[a] The equation number gives the place where the symbol appears for the first time.

4. Complete set of commuting operators

$C(C(i))$	CSCO–I, or CSCO of $G(G(i))$
$\underline{C}(s) = (C(1), C(2), \ldots)$	complete set of commuting operators of $G(s)$
$\overline{C}(s) = (\overline{C}(1), \overline{C}(2), \ldots)$	complete set of commuting operators of $\overline{G}(s)$
$C(s')$	CSCO of a non–canonical subgroup chain $G(s')$
$M = (C, C(s))$	CSCO–II of G
$K = (C, C(s), \overline{C}(s))$	CSCO–III of G
$C(n)$	CSCO–I of S_n, or the two–cycle class operator of S_n
$\mathcal{C}(n)$	CSCO–I of the state permutation group $\mathcal{S}_n$

5. Irreducible basis and matrices

$\psi_m^{(\nu)}$	$G \supset G(s)$ irreducible basis, (3-77b)
$\psi_m^{(\nu)k}, P_m^{(\nu)k}$	$G \supset G(s)$ and $\overline{G} \supset \overline{G}(s)$ irreducible basis
$D_{m\bar{m}}^{(\nu)}(R) = \langle \psi_m^\nu \vert R \vert \psi_{\bar{m}}^\nu \rangle$,	irreducible matrix of the element R, (2-95)
$\vert Y_m^{(\nu)} \rangle$	Yamanouchi basis, (4-11c)
$\vert Y_m^{(\nu)}(\omega) \rangle$	Yamanouchi basis of $S_n(\omega)$, (4-132)
$\left\vert \begin{smallmatrix}[\nu] \\ W\end{smallmatrix} \right\rangle, \left\vert \begin{pmatrix}[\nu] \\ (m)\end{pmatrix} \right\rangle$	Gel'fand basis for a unitary group, (4-84)
$\left\vert [\nu], \begin{smallmatrix}\tau[\nu_1][\nu_2] \\ m_1 m_2\end{smallmatrix} \right\rangle$	$S_n \supset S_{n_1} \otimes S_{n_2}$ basis, (4-165b)
$\left\vert [\nu], \begin{smallmatrix}\tau[\nu_1][\nu_2] \\ W_1 W_2\end{smallmatrix} \right\rangle$	$SU_{mn} \supset SU_m \times SU_n$, (7-106) $SU_{m+n} \supset SU_m \otimes SU_n$ basis, (7-141)
$\psi_{\mathbf{k}} = \exp[i(\mathbf{k} + \mathbf{K}_m) \cdot \mathbf{r}]$	irreducible basis of the lattice group

6. Coefficients

$C^{(\nu)\tau,m}_{\nu_1 m_1, \nu_2 m_2}$,	CG coefficients, (3-282)
$C^{(\nu)\tau,m}_{\nu_1 m_1, \nu_2 m_2, \omega}$,	induction coefficients of S_n, (4-140)
$\left[\begin{smallmatrix} \nu \mathbf{k} \nu' \mathbf{k}' \\ \sigma a \sigma' a' \end{smallmatrix} \middle\vert \begin{smallmatrix} \nu'' \mathbf{k}'' \theta \\ \sigma'' a'' \end{smallmatrix} \right]$,	CG coefficients for space groups, (10-138a)
$C^{(\nu)\tau,\beta\Lambda}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2}$,	$G \supset G_1$ isoscalar factor (ISF), (3-302)
$C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'}$,	$S_n \supset S_{n-1}$ ISF, (4-188)
$C^{[\nu]\theta,[\nu']\theta'}_{\nu_s\nu'_s,\nu_t\nu'_t} = \langle \nu_s \nu_t, \nu \vert b^\dagger \vert \nu'_s \nu'_t, \nu' \theta' \rangle$,	$S_n \supset S_{n-1}$ ISF, (9-18)
$C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'}$,	$S_n \supset S_{n-1}$ outer–product ISF, (7-252)
$C^{[\nu]\beta,[\nu']\beta'}_{\nu_1\nu'_1,\nu_2\nu_2} = \langle \nu_1\nu_2, \nu \vert a_1^\dagger \vert \nu'_1\nu_2, \nu'\beta' \rangle$,	$S_n \supset S_{n-1}$ outer–product ISF,(9-14b)
$C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\varphi\mu'\mu''}$	$S_n \supset S_{n_1} \otimes S_{n_2}$ ISF, (4-200) $S_n \supset S_{n_1} \otimes S_{n_2}$ outer–product ISF, (7-265)
$C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''}$,	$SU_{mn} \supset SU_m \times SU_n$, (7-224a)

	$SU_{m+n} \supset SU_m \otimes SU_n$ ISF, (7-268)
$C^{[\nu]\tau,\alpha L}_{[\nu_1]\alpha_1 L_1,[\nu_2]\alpha_2 L_2}$,	$SU_{2l+1} \supset SO_3$ ISF (or CFP), (7-166)
$C^{[\nu]\tau,\beta ST}_{[\nu_1]\beta_1 S_1 T_1,[\nu_2]\beta_2 S_2 T_2}$,	$SU_4 \supset SU_2 \times SU_2$ ISF (or CFP), (7-176)
$\left\langle \begin{matrix}[\nu]\\ m\end{matrix} \middle\| [\nu], \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1 m_2\end{matrix} \right\rangle$, or $\langle [\nu]m \| \tau[\nu_2]m_2\rangle$,	subduction coefficients (SDC) of S_n, (4-168a)
$\left\langle \begin{matrix}[\nu]\\ w\end{matrix} \middle\| [\nu], \begin{matrix}\tau[\nu_1][\nu_2]\\ w_1 w_2\end{matrix} \right\rangle$,	$SU_{mn} \downarrow (SU_m \times SU_n)$ SDC,(7-115) $SU_{m+n} \downarrow (SU_m \otimes SU_n)$ SDC, (7-144)
$P^{(\nu)k}_m = \sqrt{\frac{h_\nu}{g}} \sum_a D^{(\nu)*}_{mk}(R_a) R_a$	normalized projection operator, (3-199)
$P^{(\nu)}_{mk} = \frac{h_\nu}{g} \sum_a D^{(\nu)*}_{mk}(R_a) R_a$	projection operator, (3-222)
$P^{(\nu)} (= \sum_m P^{(\nu)}_{kk})$	projection operator, (3-51), (3-233)
$R^{[\nu]k}(\omega)$,	normalization coefficients, (4-81a)

7. Miscellaneous

$C_i, C(\varphi)$	class operators
$\tilde{C}_{jm} = (-1)^{j+m} C_{j-m}$	time reversal state
$\tilde{D}$	the transpose of the matrix D
$\varepsilon_i(\nu_1 \nu_2 \nu)$	phase factor
Λ^ν_m	phase of the Yamanouchi basis vector
$\Lambda^\nu_{\nu'}$	relative phase of Yamanouchi basis vectors, (4-196')
$h_\nu, \|\nu\|$	dimension of the irrep ν
$\hat{j} = \sqrt{2j+1}$	
$g, \|G\|, \|\mathbf{G}\|$	order of a group
g_i	number of elements in the class i
N	number of classes
ν_0	the adjoint rep

8. Abbreviations

CAR	Cartesian representation
CG coefficients	Clebsch–Gordan coefficients
CFP	coefficients of fractional parentage
CSCO	complete set of commuting operators
CSW	complete set of weights
DYN	Dynkin representation
EFM	eigenfunction method
FWS	fundamental weight system representation
IDC	induction coefficients of permutation group, or outer-product reduction coefficients
irrep	irreducible representation
IRB	irreducible basis
ISF	isoscalar factor
rep	representation
SALC	symmetry adapted linear combination
SDC	subduction coefficients
SRS	simple roots representation

The main notations for the space group are listed below:

Genealogical relation for the space group and its point groups

$$\mathbf{G} \supset \mathbf{G}(\mathbf{k}) \supset \mathbf{G}(s) \supset \mathbf{T} ,$$
$$\mathbf{P} \supset \mathbf{G}_0 \supset \mathbf{G}_0(\mathbf{k}) ,$$
$$\mathbf{P} \supset \mathbf{P}(\mathbf{k}) ,$$
$$\mathbf{G}_0(\mathbf{k}) = \mathbf{P}(\mathbf{k}) \cap \mathbf{G}_0$$

Coset decomposition

$$\mathbf{G} = \sum_{\sigma}^{q} \oplus \{\beta_\sigma|\mathbf{V}_\sigma\}\mathbf{G}(\mathbf{k}) ,$$
$$\mathbf{G}_0 = \sum_{\sigma}^{q} \oplus \beta_\sigma \mathbf{G}_0(\mathbf{k})$$

Table 1. Space-group elements, IRB and irrep.

	$\mathbf{G}$	$\mathbf{G}(\mathbf{k})$[a]	$\mathbf{T}$	$\mathbf{G}'^{b}_{\mathbf{k}}$	$\mathbf{G}_0(\mathbf{k})$[c]
group element	$\{\alpha_i\|\mathbf{V}(\alpha_i)+\mathbf{R}_n\}$	$\{\gamma_i\|\ \mathbf{V}(\gamma_i)+\mathbf{R}_n\}$	$\{\varepsilon\|\mathbf{R}_n\}$	$\{\gamma_i\|\mathbf{V}(\gamma_i)\}'$	γ
basis vector	$\psi^{(\nu)}_{\mathbf{k}_\sigma a} = \{\beta_\sigma\|\mathbf{V}_\sigma\}\psi^{(\nu)}_{\mathbf{k},a}$	$\psi^{(\nu)}_{\mathbf{k},a}$	$\psi_{\mathbf{k}} = e^{i(\mathbf{k}+\mathbf{K}_m)\cdot r}$	$\psi^{(\nu)}_{\mathbf{k},a}$	
irrep	$D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}$	$D^{(\mathbf{k})(\nu)}_{ba}$	$\exp(-i\mathbf{k}\cdot\mathbf{R}_n)$	$D^{(\mathbf{k})(\nu)}_{ba}$	$\Delta^{(\nu)}_{ba}$
dimension	qh_ν	h_ν	1	h_ν	h_ν

[a]The irrep of $\mathbf{G}(\mathbf{k})$ is $D^{(\mathbf{k})(\nu)}(\{\gamma|\mathbf{c}\}) = \exp(-i\mathbf{k}\cdot\mathbf{c})\Delta^{(\nu)}(\gamma)$.

[b]$\{\gamma_j|\mathbf{V}(\gamma_j)\}' = R_j = \exp[i\mathbf{k}\cdot\mathbf{V}(\gamma_j)]\ \{\gamma_i|\mathbf{V}(\gamma_i)\}$, $j = 1,2,\ldots,|\ \mathbf{G}_0(\mathbf{k})\ |$, are the active elements of the rep group $\mathbf{G}'_{\mathbf{k}}$.

[c]$\Delta^{(\nu)}$ is the projective irrep of the little co-group $\mathbf{G}_0(\mathbf{k})$. In full we have $\Delta^{(\nu)}(\gamma) = D^{(\mathbf{k})(\nu)}(\{\gamma|\mathbf{V}(\gamma)\}')$.

Introduction

Group theory plays a very important role in physics and chemistry, and its importance continues to grow seemingly endlessly. The representation theory of both finite and compact Lie groups is treated extensively in numerous books and articles. However, they basically follow the same fundamental theory. This theory, which we call the standard group representation theory, seems to be perfect from the mathematical point of view. Nevertheless, it is not totally satisfying from a practical or physical point of view. Many sophisticated physicists, who were quite at home in their own fields, seemed to be afraid of group theory and expressed their dissatisfaction with standard representation theory (Sokolov 1956, Salam 1963, Lipkin 1966, Slater 1975). During the 1930's–50's, outrage, disgust, characterizing group theory as a plague or calling it "*Gruppenpest*" were not atypical reactions by physicists to the use of group theory in physics. The leading American physicist J. Slater commented (p. 60 in his autobiography):

"*The authors of the 'Gruppenpest' wrote papers which are incomprehensible to those like me who had not studied group theory, in which they applied these theoretical results to the study of many electron problem. The practical consequences appeared to be negligible, but everyone felt that to be in the mainstream one had to learn group theory. Yet there were no good texts for which one could learn group theory. It was a frustrating experience, worthy the name of a pest. I had what I can only describe as a feeling of outrage at the turn which the subject had taken....*

As soon as this [Slater's] paper became known, it was obvious that a great many other physicists were disgusted as I had been with the group theoretical approach to the problem. As I heard later, there were remarks made such as 'Slater has slain the Gruppenpest'. I believe that no other piece of work I have done was so universally popular."

The Nobel Laureate A. Salam said in his opening speech for "Seminars on Theoretical Physics" held in Trieste in 1962:

"*In 1951, I had the good fortune of listening to Professor Racah's lecture on Lie groups at Princeton. After attending these lectures, I thought, "This is really too hard. I cannot learn all this ... All this is too damned hard and unphysical.*"

Despite those comments being made several decades ago, and despite group theory being now a more common part in the education of physicists, significant difficulties with the standard representation theory of groups have not been overcome. There lacks the universal applicability and acceptability associated with, for example, calculus.

The first serious drawback of the standard group representation theory is that it is *unphysical*. By this I mean it was developed by mathematicians for mathematical purposes and without physical application in mind. The group was introduced into mathematics as early as 1810, and the theory of group representation was developed during the 1920's, before quantum mechanics was formulated; in this respect it is unlike calculus, which was invented about the same time as Newton's laws were discovered. Second, there is no general method for treating various kinds of group representation problems. Any given technique applies only to a particular problem and for a particular group, or class of groups. Not only do many of the methods for dealing with point groups, permutation groups, space groups, and Lie groups all differ drastically from each other, but the methods for finding the characters, irreducible basis (IRB), irreducible matrices and Clebsch–Gordan (CG) coefficients also vary from one to the other. Therefore, in many cases, these methods are more of an art than a science. Third, in physical applications, we often need

to construct an IRB $\psi_m^{(\nu)}$ symmetry adapted to a given group chain $G \supset G(s)$. The standard method is to use the projection operator

$$P_{mk}^{(\nu)} = \frac{h_\nu}{g} \sum_R D_{mk}^{(\nu)}(R)^* R,$$

where $D^{(\nu)}(R)$ are irreducible matrices in the $G \supset G(s)$ IRB, which in turn depend on the $G \supset G(s)$ IRB $\psi_m^{(\nu)}$ through the relation

$$D_{mk}^{(\nu)}(R) = \langle \psi_m^{(\nu)} | R | \psi_k^{(\nu)} \rangle.$$

Now the trouble is that the $G \supset G(s)$ IRB is not known yet. Thus we are at an impasse when both the matrices and IRB are unknown.

As pointed out by Salam (1963), a battle has raged between the amateurs and professional group theorists. The amateurs have maintained that everything one needs from the theory of groups can be discovered by the light of nature provided one knows how to multiply two matrices. As an amateur myself, in this book I have introduced a new (certainly, non–professional) approach to group representation theory and it is quite interesting to note that the foundation of the new approach is precisely the theory of the complete set of commuting operators (CSCO) initiated by Dirac, the prince of amateurs in the field of group theory.

The special features of the approach are as follows.

1. *Simplicity and Accessibility*: The new representation theory for groups is essentially an extension of representation theory in quantum mechanics. Group representation theory is intimately related to quantum mechanics just as calculus is to classical mechanics. Thus it should be easily acceptable to physicists. For a group G, three kinds of CSCO are introduced, the CSCO–I, –II, and –III, roughly speaking the CSCO for the class space, the irreducible space, and the group space, respectively. They are the analogies of $\mathbf{J}^2$, $(\mathbf{J}^2, J_z)$, $(\mathbf{J}^2, J_z, J_3)$, respectively, for the rotation group in three–dimensional space.

2. *Universality and Versatility*: Based on the CSCO–I, –II, and –III, all compact (discrete or continuous) groups are treated in a unified way. Therefore once one knows the representation theory of the rotation group, in principle one knows the representation theory of all other compact groups. The new approach is constructive in nature, leading to a new method, the so–called eigenfunction method (EFM) for determining group representation. The problems of determining firstly the primitive characters and isoscalar factors, secondly the $G \supset G(s)$ IRB and CG coefficients, and thirdly the irreducible matrices, are all reduced to a single recipe: Seek the eigenvectors (or eigenfunctions) of the CSCO–I, –II, and –III of G, respectively. The EFM proves to be powerful and versatile in treating point groups, permutation groups, unitary groups, graded unitary groups and space groups, and for both vector and projective representations. The EFM for a discrete group (both for finite and infinite types) is simpler than conventional methods and is flexible enough to obtain the irreducible basis adapted to any given group chain $G \supset G(s)$ without need of any knowledge of the irreducible matrices, or conversely, to obtain all the irreducible matrices in any given $G \supset G(s)$ classification without any knowledge of the irreducible basis.

3. *Applicability*: Since the ultimate step of the method is the diagonalization of the representative matrices of a certain type of CSCO, the procedure can be easily translated into a computer program. Several standard codes are already available. Furthermore, using the eigenvalues of the CSCO as irrep labels enables us to find *algebraic solutions* for the point groups, just as one has analytic solutions for rotation group.

The book is self–contained and suitable for self–study, and is a combination of a textbook and a monograph. By ignoring some proofs and some paragraphs or passages marked with asterisks, the book becomes an easily readable textbook. The theory is developed starting with concrete examples and leading up to more abstract conclusions, as well as from the special to the general, supplemented with abundant illustrative examples. The emphasis is on the EFM

technique rather than on strict rigor. Some theorems are cited without proof, since the theorems are easily understandable and their proofs can be found in many group theory textbooks. A knowledge of elementary group theory is not necessary to read this book, but a knowledge of the linear algebra and representation theory as well as angular momentum theory in quantum mechanics is assumed.

The various important coefficients, such as the Clebsch–Gordan, Racah, subduction and induction coefficients, the isoscalar factors and fractional parentage coefficients are discussed in detail for point groups, permutation groups, unitary groups and space groups. Tables for several useful coefficients are given. Some new dualities between the permutation group and unitary groups are disclosed and are fully exploited for computing many coefficients of unitary groups in terms of those of the permutation groups. The theory on roots and weights in Lie groups is also reformulated in the spirit of representation theory of quantum mechanics. The applications of group theory in quantum mechanics are discussed with emphasis on application to many-body systems. The connection between the new and standard approaches is discussed. There should be no difficulty for a reader of the present book to understand the conclusions derived in other textbooks or in the literature, although the derivations given here may be totally different.

Tables and figures are indexed according to their section numbers. For example, Table(Fig.) x.y-n denotes the n–th table (figure) in Sec. x.y. If there is only a single table or figure in the section, then the suffix "-1" will be omitted. References are indicated by the names of the first author, or first two authors, followed by the year of publication; if this is still not sufficient, then an index $[x]$ will precede the year.

Chapter 1

Elements of Group Theory

In this chapter we present an introduction to the basic elements of group theory. Many books are available covering the material presented herein, and we therefore state most results without references. We have found the texts of Hamermesh (1962) and Elliott & Dawber (1979) particularly useful.

1.1. The Definition of a Group

A set of elements (or operators) $\{a, b, c, \ldots\}$ or $\{R_a : a = 1, 2, 3, \ldots\}$, or $\{R, S, T, \ldots\}$ is called a group G , if a multiplication rule is defined for any two elements so that the product ab has a definite meaning and the following four postulates are satisfied:

1. *Closure*: If a and b belong to the set, then ab also belongs to the set.
2. *Associativity*: $a(bc) = (ab)c$.
3. There exists the identity element e such that $ae = ea = a$ for any a belonging to the set.
4. There exists the inverse element, that is, for each element a, there is a corresponding element b such that $ab = ba = e$. b is called the inverse element of a and denoted by $b = a^{-1}$.

Since in general $ab \neq ba$ the order of multiplication is important. An *Abelian group* is one whose elements commute with one another, that is $[a, b] = ab - ba = 0$.

A *finite group* has a finite number of elements. For some infinite groups, called *continuous groups*, the group elements may be labelled by parameters which (or some of which) vary continuously.

We use $G = \{a\}$ to denote a group, and use $a \in G$ to denote that a is an element of G (read as a belongs to G). The *order of a finite group* G is defined as the total number of its elements and will be denoted by g or $|G|$.

For a finite group, $a^n = e$ for some positive integer n and each $a \in G$. The smallest positive n for which $a^n = e$ is called the *order of the element* a , and denoted as $|a|$. The set of elements $a, a^2, a^3, \ldots, a^n (= e)$ forms a group, called the *cyclic group* of order $n = |a|$, which is often denoted by C_n.

A set of *generators* of a group G is a set of elements $\{a, b, c \ldots\}$ of G such that every element of G is expressible as a finite product of powers of elements of $\{a, b, c, \ldots\}$.

From a mathematical point of view, the product ab of two elements a and b can be defined arbitrarily. In physics, we are mainly interested in the group of transformations, or the group of operators. In such cases, the group elements $R_a, R_b \ldots$ represent a transformations or operators, and the product $R_a R_b = R_c$ is defined as the operation resulting from first operating with R_b and then with R_a.

Definition 1.1: Two sets S and S' are said to be commutative, denoted by $[S, S']$=0, if each element of S commutes with each element of S'.

All the operations which leave a system (or a geometric object) unchanged (that is it appears not to have changed after the operation) form a group called the *symmetry group* of the system (or the object).

Obviously, the Hamiltonian H of a microscopic system commutes with the symmetry group G of the system, that is

$$[H, G] = 0 \,. \tag{1-1a}$$

According to Definition 1.1, this means that

$$[H, R_a] = 0 \quad \text{for } R_a \in G \,. \tag{1-1b}$$

Examples of groups:

1. All the integers under addition form an infinite discrete group.
2. The integers modulo n (that is $a = b$ if $a - b = mn, m$ being an integer) under addition form a group called the *group of integers modulo n* and denoted as Z_n.
3. The n complex numbers $\exp(2\pi mi/n), m = 0, 1, \ldots, n-1$ form the cyclic group C_n under multiplication.

   The three previous groups are Abelian, the following group is non–Abelian.
4. The rotation group R_3 in three dimensions: A system with spherical symmetry is invariant under rotations through any angle φ about any axis $\mathbf{n}(\theta', \varphi')$ passing through its center. All these operations

$$R_{\mathbf{n}(\theta',\varphi')}(\varphi), \quad 0 \le \theta' \le \pi, \quad 0 \le \varphi' \le 2\pi, \quad 0 \le \varphi \le \pi \tag{1-2a}$$

   form the three-dimensional rotation group R_3. The identity is $R_{\mathbf{n}}(0)$, and the inverse of $R_{\mathbf{n}(\theta',\varphi')}(\varphi)$ is

$$R^{-1}_{\mathbf{n}(\theta',\varphi')}(\varphi) = R_{\mathbf{n}(\pi-\theta',\pi+\varphi')}(\varphi) \,. \tag{1-2b}$$

   Since θ', φ' and φ are continuous variables, and two rotations do not in general commute, R_3 is a continuous non–Abelian group.
5. The rotation group R_2 in two dimensions: A linear molecule such as CO is invariant under rotations through any angle about the axis z passing through the line connecting the centers of the atoms. The symmetry operations are

$$R_z(\varphi), \quad 0 \le \varphi \le 2\pi \,. \tag{1-2c}$$

   Together they form the two-dimensional rotation group R_2. It is clear that

$$R_z(\varphi_1)R_z(\varphi_2) = R_z(\varphi_2)R_z(\varphi_1) = R_z(\varphi_1 + \varphi_2) \,;$$

   so that R_2 is a continuous Abelian group.
6. Space inversion group G_I or C_i consists of two elements: the identity e and the space inversion I which takes the point $P(x, y, z)$ to $P'(-x, -y, -z)$.
7. Space reflection group C_s consists of two elements: the identity e and the space reflection σ_z, a reflection plane in the xy plane (with z as its normal) which takes the point $P(x, y, z)$, to $P'(x, y, -z)$.
8. The group C_{3v}: The ammonia molecule NH_3 (Figs. 1.1-1a and 1.1-1b) has six symmetry operations,

$$e, C_3, C_3^2, \sigma_1, \sigma_2, \sigma_3 \,, \tag{1-3}$$

   where $C_3 = R_z(120°), C_3^2 = R_z(240°)$, and σ_i are reflection planes containing the z–axis and the vertices i, as shown in Fig. 1.1-1b. The six operations in Eq. (1-3) form the symmetry group of NH_3, denoted as C_{3v}.

   Using the interchange of the vertices 1, 2, 3 under the operations (1-3), we can obtain the multiplication table for C_{3v}. Note that the anti–clockwise rotation is taken to be positive,

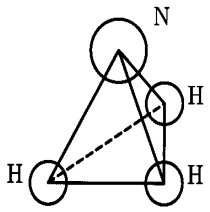


Fig. .1.1-1a. The ammonia molecule NH_3 with C_{3v} symmetry.

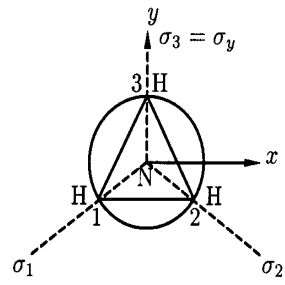


Fig. 1.1-1b. The ammonia molecule NH_3 seen from the top

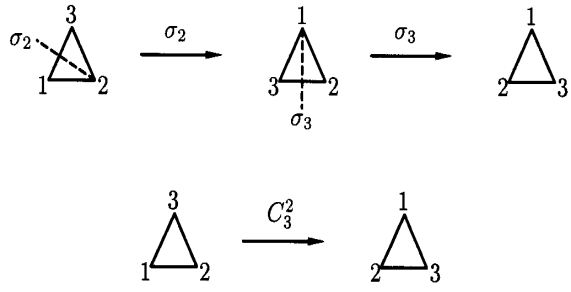


Fig. 1.1-2. Reflections and rotations on a triangle.

and the reflection planes σ_i are fixed in space (that is they do not change with the vertices). Consider for example the sequence shown in Fig. 1.1-2.

Hence we see that $\sigma_3\sigma_2 = C_3^2$. The multiplication relations for the elements of C_{3v} is listed in Table 1.1. Such a table is called a group table.

10. An arbitrary quaternion can be written as

$$q = q^0\lambda_0 + q^1\lambda_1 + q^2\lambda_2 + q^3\lambda_3$$

The q^i are real and λ_i obey

$$\lambda_0\lambda_i = \lambda_i,\ \lambda_i^2 = -\lambda_0,\ i = 1,2,3;$$
$$\lambda_i\lambda_j = -\lambda_j\lambda_i,\ \lambda_i\lambda_j = \lambda_k,\ i,j,k \text{ cyclic.} \tag{1-4a}$$

(when $q_3 = q_4 = 0$, a quaternion is reduced to a complex number). The quaternions $\pm\lambda_0, \cdots, \pm\lambda_3$ form a group under multiplication($e = \lambda_0$), called the *quaternion group Q* .

9. If a set of matrices constitutes a group under matrix multiplication, then it is called a *matrix group*. For example, one realization of the quaternions is

$$\lambda_0 = \{1,1\}_{\text{diag}},\ \lambda_1 = -i\sigma_x,\ \lambda_2 = -i\sigma_y,\ \lambda_3 = -i\sigma_z,$$

where σ_x, σ_y and σ_z are the Pauli matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1-4b}$$

The eight matrices $\{\pm e, \pm i\sigma_x, \pm i\sigma_y, \pm i\sigma_z\}$ from a matrix group

Ex. 1.1. Show that the elements in the same class have the same order.

Ex. 1.2. Prove that if two elements a and b commute, then a^{-1} and b also commute.

Table 1.1. The group table of C_{3v}.

ab \ b / a	e	σ_3	σ_2	σ_1	C_3	C_3^2
e	e	σ_3	σ_2	σ_1	C_3	C_3^2
σ_3	σ_3	e	C_3^2	C_3	σ_1	σ_2
σ_2	σ_2	C_3	e	C_3^2	σ_3	σ_1
σ_1	σ_1	C_3^2	C_3	e	σ_2	σ_3
C_3	C_3	σ_2	σ_1	σ_3	C_3^2	e
C_3^2	C_3^2	σ_1	σ_3	σ_2	e	C_3

Ex. 1.3. Check the multiplication relations in Table 1.1.

Ex. 1.4. Construct the multiplication table for the quaternion group (1-4a).(Hint: a 4×4 table is sufficient.)

Ex. 1.5. Construct the group table for the group C_{4v} which consists of the following eight elements: $\{e, C_4, C_4^2, C_4^3, \sigma_1, \sigma_2, \sigma_3, \sigma_4\}$, where $C_4 = R_z(90°)$, and σ_i are reflection planes shown in Fig. 1.1-3.

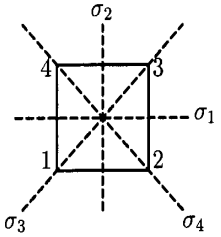


Fig. 1.1-3. The group C_{4v}.

1.2. The Permutation Group S_n

1.2.1 The definition of S_n

The $n!$ permutations

$$\begin{pmatrix} 1, & 2, & \dots & n \\ p_1, & p_2, & \dots & p_n \end{pmatrix} \equiv \begin{pmatrix} i \\ p_i \end{pmatrix} \tag{1-5}$$

form a group $S_n(1, 2, \dots, n) \equiv S_n$, called the *permutation group* or the *symmetric group*. Equation (1-5) denotes a permutation of the indices i to p_i. The product $R_1 R_2$ of two permutations is defined as the resultant permutation of first permuting with R_2 and then with R_1. For example,

$$R_1 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}, \quad R_2 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix},$$

$$R_1 R_2 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix},$$

$$R_2 R_1 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}.$$

One can show that for general permutations R_1 and R_2

$[R_1, R_2] = 0$, if R_1 and R_2 do not involve the permutation of the same index,

$[R_1, R_2] \neq 0$, if R_1 and R_2 involve the permutation of the same index. Obviously we have that

$$\begin{pmatrix} 1 & 2 & 3 \\ p_1 & p_2 & p_3 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 3 \\ p_2 & p_1 & p_3 \end{pmatrix} = \begin{pmatrix} 3 & 2 & 1 \\ p_3 & p_2 & p_1 \end{pmatrix} = \dots$$

and that the inverse of $\begin{pmatrix} i \\ p_i \end{pmatrix}$ is $\begin{pmatrix} p_i \\ i \end{pmatrix}$. Consider for example the permutation group S_3 with the following 3!=6 permutations:

$$R_1 = e = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix}, R_2 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}, R_3 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix},$$

$$R_4 = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix}, R_5 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}, R_6 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}. \tag{1-6}$$

1.2.2. Permutations expressed in terms of cycles and transpositions

Define:

$$\begin{aligned} e &= (i), && \text{one-cycle} \quad (i \text{ remains } i), \\ p_{ij} &= (ij) = \begin{pmatrix} ij \\ ji \end{pmatrix}, && \text{two-cycle, or transposition,} \\ p_{ijk} &= (ijk) = \begin{pmatrix} ijk \\ jki \end{pmatrix}, && \text{three-cycle.} \end{aligned}$$

Similarly, $(p_1, p_2 \dots p_k)$ is called a k-cycle and k is called the *length* of the cycle. A k-cycle $(p_1, p_2 \dots p_k)$ generates the cyclic group C_k.

Any permutation can be expressed as a product of cycles without common indices

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 4 & 3 & 7 & 1 & 5 & 8 & 2 & 6 \end{pmatrix} = (14)(237)(5)(68)\,. \tag{1-7}$$

Remarks:

1. In expressing a permutation as a product of cycles without common indices, the order with which we write the cycles is irrelevant.

2. One-cycles can be omitted. Hence the permutation (1-7) can be written as (14) (237) (68).

3. A cycle can be written in several forms, since it is itself invariant under cyclic permutations. For example

$$(\alpha\beta\gamma\delta) = (\beta\gamma\delta\alpha) = (\gamma\delta\alpha\beta) = (\delta\alpha\beta\gamma).$$

Any transposition can be expressed as a product of adjacent transpositions by the following recursive formula:

$$(i, i+v) = (i+1, i+v)(i, i+1)(i+1, i+v). \tag{1-8a}$$

Example 1: The group S_4. Letting $v = 2$ in (1-8a),

$$(13) = (23)(12)(23), \quad (24) = (34)(23)(34). \tag{1-8b}$$

Letting $v = 3$ in (1-8a) and using (1-8b),

$$(14) = (24)(12)(24) = (34)(23)(34)(12)(34)(23)(34). \tag{1-8c}$$

The following important relations can be verified:

$$1.\ (\alpha\beta\gamma\delta\varepsilon) = (\alpha\beta)(\beta\gamma\delta\varepsilon) = (\alpha\beta\gamma)(\gamma\delta\varepsilon) = (\alpha\beta\gamma\delta)(\delta\varepsilon) = (\alpha\beta)(\beta\gamma)(\gamma\delta)(\delta\varepsilon). \tag{1-9a}$$

$$2.\ (\alpha\beta\gamma\delta\varepsilon) = (\alpha\varepsilon)(\alpha\beta\gamma\delta) = (\alpha\delta\varepsilon)(\alpha\beta\gamma) = (\alpha\gamma\delta\varepsilon)(\alpha\beta) = (\alpha\varepsilon)(\alpha\delta)(\alpha\gamma)(\alpha\beta). \tag{1-9b}$$

$$3.\ (\alpha\beta\gamma\delta\varepsilon)^{-1} = (\alpha\varepsilon\delta\gamma\beta) = (\varepsilon\delta\gamma\beta\alpha). \tag{1-10}$$

Note that the order of the cycles in the above equations is crucial, since they involve common indices.

The *generators* of S_n are the $n-1$ adjacent transpositions $(i, i+1), i = 1, 2, \ldots, n-1$.

A permutation can be written as a product of transpositions in many ways but the number N of factors is always even or odd. Therefore for any permutation p, we can define a *permutation parity*, or *sign*, δ_p by

$$\delta_p = (-1)^N. \tag{1-11}$$

A permutation with $\delta_p = 1(-1)$ is called an even (odd) permutation. If $p = p_1 p_2$, then $\delta_p = \delta_{p_1}\delta_{p_2}$. The k–cycle $(i_1 i_2 \ldots i_k)$ has parity $(-1)^{k-1}$.

Example 2: The six elements (1-6) of S_3 can be written in terms of cycles as

$$R_1 = e, \quad R_2 = (12), \quad R_3 = (13), \quad R_4 = (23), \quad R_5 = (123), \quad R_6 = (132), \tag{1-12}$$

where e, (123) and (132) are even, while (12), (13) and (23) are odd. The group table of S_3 is shown in Table 1.2.

Table 1.2 Group table of S_3. Subscripts record the permutation column/row number.

$a = cb$ (b / c)	e_1	$(12)_2$	$(13)_3$	$(23)_4$	$(123)_5$	$(132)_6$
e_1	e_1	$(12)_2$	$(13)_3$	$(23)_4$	$(123)_5$	$(132)_6$
$(12)_2$	$(12)_2$	e_1	$(132)_6$	$(123)_5$	$(23)_4$	$(13)_3$
$(13)_3$	$(13)_3$	$(123)_5$	e_1	$(132)_6$	$(12)_2$	$(23)_4$
$(23)_4$	$(23)_4$	$(132)_6$	$(123)_5$	e_1	$(13)_3$	$(12)_2$
$(123)_5$	$(123)_5$	$(13)_3$	$(23)_4$	$(12)_2$	$(132)_6$	e_1
$(132)_6$	$(132)_6$	$(23)_4$	$(12)_2$	$(13)_3$	e_1	$(123)_5$

1.3. Subgroups

If there is a subset of elements in a group G, which by itself forms a group G_s under the same multiplication rule as that of G, then G_s is said to be a *subgroup* of G, denoted by $G \supset G_s$. Every group has two trivial subgroups, called *improper subgroups*: the group consisting of the identity element alone, and the whole group itself. All other subgroups are called *proper subgroups*.

A subgroup G_s may itself contain a subgroup G'_s. Together they form a group (or subgroup) chain,

$$G \supset G_s \supset G'_s \supset \ldots .$$

Examples of subgroups:

1. $R_3 \supset R_2$. The two–dimensional rotation group is a subgroup of the three-dimensional rotation group.

2. The group $\mathcal{C}_{3v}$ has four subgroup chains, namely

$$\mathcal{C}_{3v} \supset C_3, \quad \mathcal{C}_{3v} \supset \mathcal{C}_{s_i}, \quad i = 1,2,3$$

$$C_3 = (e, C_3, C_3^2), \quad \mathcal{C}_{s_i} = (e, \sigma_i).$$

3. The group S_n has the group chain $S_n \supset S_{n-1} \supset S_{n-2} \supset \ldots \supset S_2$.
4. The group S_4 has a variety of other subgroups, for example $S_3(134)$, $S_3(234), \ldots$ as well as the following two Abelian subgroups:

$$\text{the Four-group:} \quad F = \{e, (12)(34), (13)(24), (23)(14)\}\,, \tag{1-13}$$

$$\text{the cyclic group:} \quad \mathcal{C}_4 = \{e, (1234), (1234)^2 (= (13)(24)), (1234)^3\}\,. \tag{1-14}$$

5. The *alternating group* $\mathcal{A}_n$ is the group consisting of all the even permutations of S_n.

Ex. 1.6. Prove the following theorem: A group without any nontrivial subgroup is a group of prime order.

Ex. 1.7. Using (1-9) check Table 1.2.

Ex. 1.8. Construct the group table for the four-group.

1.4. Isomorphism and Homomorphism

Two groups G and G' are said to be *isomorphic*($G \approx G'$) if their elements can be put into a one-to-one correspondence which preserves the multiplication rule, that is, corresponding to $ab = c$, we have $a'b' = c'$.

Two groups are said to be *anti-isomorphic* if their elements have a one-to-one correspondence and corresponding to $ab = c$ we have $b'a' = c'$ (instead of $a'b' = c'$).

If $ab = c$, then $b^{-1}a^{-1} = c^{-1}$. Letting $R_a = a^{-1}, R_b = b^{-1}, \ldots$ then the set $\{R_a\}$ forms a group $\tilde{G}$ which is isomorphic with G'. The difference between the group $\tilde{G}$ and G is merely a matter of nomenclature for the elements. Therefore, if G is anti-isomorphic to G', then essentially G is isomorphic to G'.

Two groups which are isomorphic are the same abstract group, though they may have totally different realizations. Therefore, we sometimes simply use $G = G'$ to indicate that G is isomorphic to G'.

Example 1: The group of integers modulo n, Z_n, is isomorphic to the cyclic group C_n.
Example 2: From Tables 1.1 and 1.2 one sees that $\mathcal{C}_{3v}$ is isomorphic to S_3:

$$\begin{array}{cccccc} e, & C_3, & C_3^2, & \sigma_1, & \sigma_2, & \sigma_3. \\ e, & (123), & (132), & (23), & (13), & (12). \end{array} \tag{1-15}$$

The isomorphism (1-15) can also be established without using the group table. First label the three vertices of a triangle in a definite way, such as ${}_1^3\Delta_2$. This is called the original triangle. Under the group operations, the vertices are interchanged among themselves. The group operator is represented by the permutation of the vertices of the original triangle. For example, under the rotation C_3.

$${}_1^3\Delta_2 \xrightarrow{C_3} {}_3^2\Delta_1\,, \quad C_3 \leftrightarrow (123)\,.$$

Thus C_3 corresponds to the permutation (123), which signifies that after the operation C_3, the vertex 1 goes to where 2 was, 2 to where 3 was, and 3 to where 1 was.

We can use this method to obtain the isomorphism (1-15). This method also applies to other point groups [see for example Eq. (3-21) and Tables 8.2-2].

Note that the correspondence $C_3 \leftrightarrow (123)$ only refers to the original triangle. For example, from

$$ {}^{3}_{1}\triangle^{2}_{2} \xrightarrow{\sigma_1} {}^{2}_{1}\triangle^{3}_{3} \xrightarrow{C_3} {}^{3}_{2}\triangle^{1} $$

one sees that the effect of the operation C_3 on the second triangle is not to move the vertex 1 to where 2 was, and so on. Summarizing, in discussing the isomorphism between $\mathcal{C}_{3v}$ and S_3, C_3 always corresponds to (123), while in discussing the effect of C_3 on a triangle, it always rotates the triangle through 120°.

Example 3: The subgroups $S_3(124), S_3(134)$ and $S_3(234)$ are all isomorphic to $S_3 \equiv S_3(123)$.

Cayley's Theorem: Every finite group G is isomorphic to a subgroup of the permutation group $S_{|G|}$.

Suppose that $R_a(R_1, R_2, \ldots, R_{|G|}) = (R_{a_1}, R_{a_2}, \ldots R_{a_{|G|}})$, which shows that the effect of multiplying the group elements of G from the left by an element R_a is a permutation of the group elements. Therefore the group element R_a corresponds to the permutation

$$ R_a \longleftrightarrow p_a = \begin{pmatrix} 1 & 2 & \ldots & |G| \\ a_1 & a_2 & \ldots & a_{|G|} \end{pmatrix}, \tag{1-16} $$

which is an element of the permutation group $S_{|G|}$. It can be shown that $p_1, p_2, \ldots, p_{|G|}$ form a group isomorphic to G.

Reading the group table horizontally, we can easily establish the isomorphism (1-16). For example from Table 1.2 we get the isomorphism of S_3 to a subgroup of S_6, that is

$$ e = e = (1)(2)(3)(4)(5)(6)\,, \qquad p_{12} = \begin{pmatrix} 123456 \\ 216543 \end{pmatrix} = (12)(36)(45)\,, $$

$$ p_{13} = \begin{pmatrix} 123456 \\ 351624 \end{pmatrix} = (13)(25)(46)\,, \quad p_{23} = \begin{pmatrix} 123456 \\ 465132 \end{pmatrix} = (14)(26)(35)\,, $$

$$ p_{123} = \begin{pmatrix} 123456 \\ 534261 \end{pmatrix} = (156)(234)\,, \quad p_{132} = \begin{pmatrix} 123456 \\ 642315 \end{pmatrix} = (165)(243)\,. \tag{1-16'} $$

Suppose that to each element a of a group G, there is an element a' in a group G'; however, there may be several elements in G mapped to the same a' in G', and if corresponding to $ab = c$, we have $a'b' = c'$, then we say that G is *homomorphic* to G', denoted as $G \to G'$. If $G \to G'$, the set of elements of G which is mapped onto the identity of G' is called the *kernel of the homomorphism* (Bacry 1977). Isomorphism is a special case of the homomorphism.

Every group has a simplest homomorphic mapping realized by letting each element of the group correspond to the identity element.

A less trivial homomorphism is $\mathcal{C}_{3v} \to S_2$. The mapping is

$$ e, C_3, C_3^2 \to e, \qquad \sigma_1, \sigma_2, \sigma_3 \to (12)\,, \tag{1-16"} $$

and the kernel is (e, C_3, C_3^2).

An isomorphism of a group with itself, that is a one–to–one correspondence between elements of the group preserving multiplication, is known as an *automorphism*. An automorphism of G can be regarded as a linear transformation in the $|G|$–dimensional vector space. All such transformations form together the group of automorphisms. If the correspondence is brought about by conjugation (see Sec. 1.5),

$$ G \to R_a G R_a^{-1}, $$

then it is called an *inner automorphism*. The inner automorphisms form a subgroup of all automorphisms. The remaining automorphisms are called the *outer automorphisms*.

An example of an automorphism is the map,

$$(e, a, a^2) \xrightarrow{\phi} (e, a^2, a),$$

for which

$$\phi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

1.5. Conjugate Classes

An element b of a group G is said to be *conjugate* to an element a if we can find an element u in G such that

$$b = uau^{-1}. \tag{1-17}$$

We refer to uau^{-1} as a *conjugate operation* on a with u. From (1-17) we have $a = u^{-1}bu$, that is, if b is conjugate to a, then a is conjugate to b. It is easy to show that if a is conjugate to b, and b is conjugate to c, then a is conjugate to c. Any element is conjugate to itself. These three properties make conjugacy an equivalence relation.

The elements conjugate to one another from a *conjugate class*, or simply a *class*. Each element of G belongs to one of the classes. The number of classes, denoted by N, is an important characteristic of the group. Designating the number of elements in the class i by g_i, we have the result $g = \sum_{i=1}^{N} g_i$.

How do we find the classes?

Method 1: Multiply the b–th column of the group table, such as Table 1.2, from the left with the element R_b^{-1}. This gives a new table where the elements in each row belong to the same class. The new table is referred to as the *class structure table.*

Method 2: Two elements which lie symmetrically with respect to the diagonal line in the group table belong to the same class.

When a class contains the inverse of all elements in the class, the class is said to be *ambivalent.*

Remarks :

1. In every group, the identity e forms a class by itself.
2. In an Abelian group, each element forms a class by itself:

$$a = uau^{-1} = uu^{-1}a = a\ .$$

Example 1: Group R_3. Suppose that there are two rotations through the same angle φ but about different axes, say z and n axes (see Fig. 1.5). These two rotations are related by

$$R_n(\varphi) = R(z \to \mathbf{n}) R_z(\varphi) R^{-1}(z \to \mathbf{n})\ , \tag{1-18}$$

where $R(z \to \mathbf{n})$ is a rotation which takes the z–axis into the $\mathbf{n}$–axis. Therefore, all rotations through the same angle φ belong to the same class.

The geometric meaning of (1-18) is that a rotation through angle φ about the axis $\mathbf{n}$ can be thought of as the net result of three rotations: first the rotation $R^{-1}(z \to \mathbf{n})$ takes the axis $\mathbf{n}$ to z, then $R_z(\varphi)$ performs a rotation through angle φ about the z–axis, and finally $R(z \to \mathbf{n})$ takes z back to $\mathbf{n}$.

All the classes of R_3 are ambivalent on account of (1-2b). The number of classes of R_3 is infinite.

Example 2: The group C_{3v} has three ambivalent classes, namely,

$$e, \quad (C_3, C_3^2), \quad (\sigma_1, \sigma_2, \sigma_3).$$

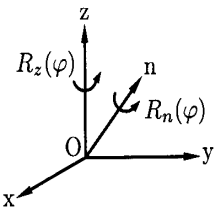


Fig. 1.5. Rotations through the same angle, but about different axes.

Example 3: Classes of the permutation group. Let $a = (ij)$ and $p = \begin{pmatrix} i \\ p_i \end{pmatrix}$ so that $p^{-1} = \begin{pmatrix} p_i \\ i \end{pmatrix}$. It is clear that

$$b = pap^{-1} = p(ij)p^{-1} = (p_i p_j),$$

since pap^{-1} represents the permutation $p_i \to i \to j \to p_j$ and $p_j \to j \to i \to p_i$, which is equivalent to $p_i \leftrightarrow p_j$. Similarly we have

$$p(ij)(klm\ldots)p^{-1} = p(ij)p^{-1}p(klm\ldots)p^{-1} = (p_i p_j)(p_k p_l p_m \ldots)\ . \tag{1-19}$$

For example, consider letting $a = (12)(345)$ and $p = (135)$. Permuting the indices in $(12)(345)$ according to what is specified by p, that is $1 \to 3 \to 5 \to 1$, we get

$$pap^{-1} = (32)(541) = (23)(154).$$

As mentioned before, in expressing a permutation by a product of independent cycles, the order of the cycle factors is irrelevant. We can always write the cycles in the order of decreasing length of the cycles. Suppose that the longest one is an i_1-cycle, the next one is an i_2-cycle $(i_1 > i_2 > \ldots)$. We can use $(i_1 i_2 \ldots)$ to represent the *cycle structure* of a permutation. The components of the cycle structure satisfy $n = i_1 + i_2 + \ldots + i_n$. For example, the cycle structure of the permutation $(237)(14)(58)(5)$ is $(3221) = (3^2 1)$ and $3 + 2^2 + 1 = 8$.

From (1-19) we know that conjugate elements of a permutation group have the same cycle structure, and vice versa. Thus elements belonging to the same class have the same permutation parity. The cycle structure can be used to write down the conjugate classes of a permutation group. For instance

Group S_3 has N=3 classes

$$\begin{aligned} &1.\ (111) = (1^3), && g_1 = 1: \ e\ . \\ &2.\ (21), && g_2 = 3: \ (12),\ (23),\ (13)\ . \\ &3.\ (3), && g_3 = 2: \ (123),\ (132)\ . \end{aligned} \tag{1-20}$$

Group S_4 has $N = 5$ classes

$$\begin{aligned} &1.\ (1^4), && g_1 = 1: \ e\ . \\ &2.\ (21^2), && g_2 = 6: \ (12),\ (13),\ (14),\ (23),\ (24),\ (34)\ . \\ &3.\ (31), && g_3 = 8: \ (123),\ (132),\ (124),\ (142), \\ & && \quad\ (134),\ (143),\ (234),\ (243)\ . \\ &4.\ (4), && g_4 = 6: \ (1234),\ (1243),\ (1324), \\ & && \quad\ (1342),\ (1423),\ (1432)\ . \\ &5.\ (2^2), && g_5 = 3: \ (12)(34),\ (13)(24),\ (14)(23)\ . \end{aligned} \tag{1-21}$$

From Eq. (1-10) one sees that the permutations a and a^{-1} have the same cycle structure, and thus belong to the same class. In other words, all classes of S_n are ambivalent classes.

Note: Two elements belonging to the same class of group G, may belong to different classes of a subgroup of G. For example, (12)(34), (13)(24) and (14)(23) belong to the same class of S_4, but each forms a class by itself for the four-group (1-13), which is a subgroup of S_4, since in the four-group we cannot find an element u such that $(12)(34) = u(13)(24)u^{-1}$.

Let us put the cycle structure in the following way

$$\underbrace{(\cdot)\cdots(\cdot)}_{f_1}\quad\underbrace{(\cdot\cdot)\cdots(\cdot\cdot)}_{f_2}\quad\underbrace{(\cdots)\cdots(\cdots)}_{f_3}\cdots,$$

that is, there are f_1 1–cycles, f_2 2–cycles,..., and f_n n–cycles, $n = \sum_{k=1}^{n} k f_k$. It can be shown (Hamermesh, 1962) that the number of the permutations of S_n which have this cycle structure is

$$g_{(f_1 f_2 \ldots)} = \frac{n!}{f_1! f_2! \ldots f_n! 2^{f_2} 3^{f_3} \cdots n^{f_n}}. \tag{1-22}$$

Letting $f_1 = n - k, f_k = 1$, and all other $f_i = 0$, we get the number of elements belonging to the k-cycle class

$$g_{(k)} = \frac{n!}{(n-k)!k} = \binom{n}{k}(k-1)! \tag{1-23}$$

where $\binom{n}{k}$ is the binary combination coefficient.

Ex. 1.9. From group Table 1.2 construct the class structure table of S_3.

Ex. 1.10. Calculate the number of elements contained in each class of S_4 and S_5.

Ex. 1.11. Find the classes of the group C_{4v}.

1.6. Cosets and Lagrange's Theorem

1.6.1 Left and right cosets

Let $H = (h_1 = e, h_2, \ldots h_{|H|})$ be a *proper* subgroup of G so that $|H| < |G|$. Suppose that a is an element of G which is not contained in H. Form the products $ah_1, ah_2, \ldots, ah_{|H|}$, and denote the set of these h elements aH. The products ah_i are all different, for if $ah_i = ah_j$, we would have $h_i = h_j$. Also none of them is contained in H, for if $ah_i = h_j$, then $a = h_j h_i^{-1}$, and a would belong to H, contrary to our assumption. If H and aH have not exhausted the group G, then we proceed as before; pick some element b of G which belongs neither to H nor to aH, and form the set bH. The set bH will again yield $|H|$ new elements of G. Continuing this process, the group G is decomposed into several disjoint sets, each containing $|H|$ elements, denoted symbolically as

$$\begin{aligned} G &= H + aH + bH + \ldots + dH \\ &= (e + a + b + \ldots + d)H \end{aligned} \tag{1-24}$$

where the plus sign "+" should be understood as the union "∪" for sets. The sets $\{aH, bH, \ldots\}$ are called the *left cosets* of H in G, and the $\{a, b, \ldots\}$ are called the *representatives* of the cosets.

Suppose that $ah_i = a_i$ for $i = 1, 2, \ldots |H|$, that is

$$aH = (a_1, a_2, \ldots, a_{|H|}), \quad a_1 = a.$$

One has that the cosets aH and $a_k H$ coincide, that is

$$aH = a_k H, \quad \text{for any } a_k \in aH,$$

since

$$a_k h_i = a h_k h_i = a h_{ki}.$$

Therefore, any element in the coset aH can be chosen as the coset representative, and for given H, the left coset decomposition of G is unique.

Analogously, we have the right coset decomposition

$$G = H + Ha' + Hb' + \ldots + Hd'. \tag{1-25a}$$

This leads to

1.6.2 Lagrange's Theorem

Lagrange's Theorem: If H is a subgroup of G, then $|H|$ divides $|G|$ so

$$|G|/|H| = m, \tag{1-25b}$$

where m is an integer and is called the *index* of the subgroup H.

From Eq. (1-25b) we immediately know that the order $|R|$ of any element R of G divides $|G|$ so that $|G|/|R|$ =integer. If $|G|$ is a prime number, then $|R|$ is necessarily either equal to one (for $R = e$) or $|G|$ (for $R \neq e$). Hence we have

Theorem 1.1: Let G be a finite group of order p where p is a prime number, then G is a cyclic group.

The left coset decomposition of S_3 is

$$\begin{aligned} S_3 &= (e + (13) + (23))[e, (12)] = (e + (123) + (132))[e, (12)] \\ &= [e, (12)] + [(13), (123)] + [(23), (132)]. \end{aligned}$$

Its right coset decomposition is

$$\begin{aligned} S_3 &= [e, (12)](e + (13) + (23)) = [e, (12)](e + (132) + (123)) \\ &= [e, (12)] + [(13), (132)] + [(23), (123)]. \end{aligned}$$

As is seen in the example above, the left cosets $a_i H$ do not in general coincide with the right cosets Ha_i.

1.6.3 Double cosets

In a manner similar to (1-24) we can partition a group G into *double cosets* with respect to the subgroups H and K,

$$G = H(e + s_2 + s_3 + \cdots + s_q)K\ , \tag{1-26a}$$

where s_i are double coset representatives. As with left and right cosets, two double cosets either coincide or have no elements in common since if $Hs_iK = Hs_\ell K$, we would have $s_i = s_\ell$. Also similar to the single coset case, any element in a double coset can be chosen as its representative. Suppose

$$HaK = \{a_{ij} :\ i = 1, \cdots, |H|; j = 1, \cdots, |K|\}\ ,\ a_{ij} = h_i a k_j,\ a_{11} = a\ .$$

Pick up another element, say $b = a_{ij}$, in HaK and form another coset

$$HbK = \{b_{\ell m} :\ \ell = 1, \cdots, |H|; m = 1, \cdots, |K|\}\ .$$

where

$$b_{\ell m} = h_\ell b k_m = h_\ell a_{ij} k_m = h_\ell h_i a k_j k_m = h_{\ell m} a h_{jm}\ .$$

Therefore $HaK = HbK$. In other words, all the elements in the same coset are on an equal footing.

There is however one essential difference between the left (or right) cosets and the double cosets. In any left (or right) coset, an element of G occurs only once, while in some double cosets an element of G may occurs more than once. We use $d(a)$ to denote the number of times, or the "frequency", that the element a occurs in the double coset HaK. It is clear that all elements in the same double coset have the same frequency, since they are on an equal footing. It can be shown (Zhang & Li, 1986) that $d(a)$ is equal to the number of elements in the intersection of the right coset Ha and the left coset aK,

$$d(a) = |a^{-1}Ha \cap K| = |Ha \cap aK| \ . \tag{1-26b}$$

A special but very useful case is when $H = K$,

$$G = H(e + s_2 + s_3 + \cdots + s_q)H \ . \tag{1-26c}$$

In applications (see Sec. 8.7), the most interesting cases are those when all $d(s_i)$ are either equal to 1 or $|H|$. According to (1-26b), $d(s_i) = 1$ when the left and right cosets s_iH and Hs_i have nothing in common except the coset generator s_i, that is when all elements in the double coset Hs_iH are distinct. On the other hand, when the left and right cosets are the same, $s_iH = Hs_i$, $d(s_i) = |H|$. For example for the identity e, $d(e) \equiv |H|$. In the case where $d(s_i) = |H|$, the double coset Hs_iH reduces to the left coset s_iH or right coset Hs_i.

Suppose that in the q double cosets, there are p cosets which are equal to single cosets. For this case the double coset decomposition (1-26c) can be re-written as

$$G = H(e + s_2 + \cdots + s_p) + H(s_{p+1} + \cdots + s_q)H \ . \tag{1-26d}$$

The decomposition (1-26d) is more convenient, since each element of G occur only once in the right cosets and double cosets. For examples and applications of the double-coset decomposition see Sec. 8.7.

1.7. Invariant Subgroups

If the left coset and the right coset of H for any element a of G are the same,

$$aH = Ha, \quad a \in G \ , \tag{1-27}$$

then we say H is an *invariant* (or *normal*) *subgroup* of G. The invariant subgroup can also be defined in the following way. If $H = (h_1, h_2, \ldots h_{|H|})$ and

$$ah_ia^{-1} \in H \ , \quad i = 1, 2, \ldots, h \ , \quad a \in G \ , \tag{1-28}$$

that is, if H is invariant under the group of inner automorphisms, then H is an invariant subgroup of G.

Equation (1-28) tells us that an invariant subgroup H contains either all or none of the elements in a class of G. The converse is also true. If a subgroup H of G consists of entire classes of G, then H is an invariant subgroup of G. Therefore, any subgroup of an Abelian group is an invariant subgroup. Thus we have the definitions

Simple group G: if $G \not\supset$ an invariant subgroup.

Semi-simple group G: if $G \not\supset$ an invariant Abelian subgroup.

where $\not\supset$ means "does not contain."

Example:

1. The group R_3 is simple, but R_2 is not.
2. The group S_3 is not semi-simple, since it contains the Abelian invariant subgroup $A_3 = (e, (123), (132))$.

The *center* of a group G is the set of elements which commute with every element of G. The center of a group G is an invariant subgroup of G.

1.8. Factor Groups*

Let H be an invariant subgroup of G. We use G/H to denote the set of cosets of H in G:

$$G/H = \{H, a_2H, \ldots, a_mH\}. \tag{1-29}$$

Define a product on the set G/H according to the rule

$$aH \times bH = abH. \tag{1-30}$$

Then the set G/H is a group under the multiplication rule (1-30), called the *factor* or *quotient group* of G relative to the invariant subgroup H. The identity of the factor group G/H is the subgroup H.

Theorem 1.2: If $G \to G'$ is a homomorphic mapping with kernel H, then H is an invariant subgroup of G and the factor group G/H is isomorphic to G'.

Proof: If $a \to e', b \to e'$, then $ab \to e'$. Also $aa^{-1} = e \to e'$ so that if $a \to e'$, then $a^{-1} \to e'$. Therefore, H is a subgroup. Since $H \to e', aH \to a'e' = a', Ha \to e'a' = a'$. Thus aH coincides with Ha, namely H is an invariant subgroup of G. Obviously, G/H is isomorphic to G'. **QED**

Example: $S_3/\mathcal{A}_3 = \{\mathcal{A}_3, \mathcal{B}\}$ is a factor group of order 2, where

$$\mathcal{A}_3 = ((e), (123), (132)), \quad \mathcal{B} = ((12), (13), (23)).$$

The multiplication relations are

$$\mathcal{A}_3\mathcal{A}_3 = \mathcal{A}_3, \quad \mathcal{B}\mathcal{B} = \mathcal{A}_3, \quad \mathcal{B}\mathcal{A}_3 = \mathcal{A}_3\mathcal{B} = \mathcal{B}\,. \tag{1-31}$$

Therefore $S_3/\mathcal{A}_3 \approx S_2$,

$$\mathcal{A}_3 \to e, \quad \mathcal{B} \to (12). \tag{1-32}$$

In the homomorphic mapping (1-32) of $S_3 \to S_2$, the kernel is $\mathcal{A}_3$, which is an invariant subgroup of S_3.

Ex. 1.12. Show that the factor group S_4/F is isomorphic to S_3.

1.9. Direct Product and Semi–Direct Product Groups

Let there be two independent (thus commuting with one another) groups $G = \{a\}$ and $G' = \{a'\}$ with different multiplication rules. Form the $|G||G'|$ pairs (a, a') (or aa') and define the product of pairs by

$$(a, a')(b, b') = (ab, a'b')\,.$$

Those $|G||G'|$ pairs form a group, called the *direct product* of G and G' and denoted $G \times G'$. From the definition, $G \times G'$ is isomorphic to $G' \times G$.

As a special case of the above, the groups G and G' can be subgroups of a larger group. For example, let G_1 and G_2 be two subgroups of G that commute with one another and let $H_i^{(1)} \in G_1, H_j^{(2)} \in G_2$

$$\left[H_i^{(1)}, H_j^{(2)}\right] = 0, \quad i = 1, \ldots, |G_1|, \quad j = 1, \ldots, |G_2|\,. \tag{1-33}$$

The $|G_1||G_2|$ products $\{H_i^{(1)}H_j^{(2)}\}$ form the direct product group $G_1 \times G_2$. $G_1 \times G_2$ is a subgroup of G. We denote this relation by $G \supset G_1 \times G_2$. Since $[G_1, G_2] = 0$, both G_1 and G_2 are invariant subgroups of $G_1 \times G_2$.

Let G be a group with subgroups G_1 and G_2 such that

1. The coset $H_i^{(2)}G_1 = G_1H_i^{(2)}$, for any $H_i^{(2)} \in G_2$,
2. Any element of G can be expressed as $R = H_i^{(1)}H_j^{(2)}$,
3. The intersection of G_1 and G_2 is the identity. The group G is called the *semi-direct product* group of G_1 and G_2, denoted by

$$G = G_1 \wedge G_2.$$

Notice that G_1 is an invariant subgroup of G, but G_2 is not necessarily invariant. In the expression $G_1 \wedge G_2$ we always write the invariant subgroup first.

Example 1: The cyclic C_6 of order 6.

$$C_6 = G_1 \times G_2, \quad G_1 = (e, a^2, a^4), \quad G_2 = (e, a^3).$$

Example 2: The group $S_n (n = n_1 + n_2)$ has two commuting subgroups $S_{n_1}(1, 2, \ldots n_1)$ and $S_{n_2}(n_1 + 1, \ldots n)$. We have $S_n \supset S_{n_1} \times S_{n_2}$.

Example 3: The rotation group R_3 commutes with the space inversion group G_I. The direct product of R_3 and G_I is called the *orthogonal group* in three-dimensional space. It is written as

$$O_3 = R_3 \times G_I.$$

Example 4: $A_3 = (e, (123), (132))$ is an invariant subgroup of S_3. The permutation group S_3 is a semi-direct product of A_3 and S_2,

$$S_3 = A_3 \wedge S_2. \tag{1-34}$$

Example 5: $S_4 = F \wedge S_3, F$ being the four-group.
Most point groups are semi-direct product groups, see (8-27).

The notion of direct or semi-direct products seems to be like an inverse to the notion of factor group. The exact relationship is follows.

1. If $G = G_1 \times G_2$, then $G/G_1 = G_2$, and $G/G_2 = G_1$.
2. If $G = G_1 \wedge G_2$, then $G/G_1 = G_2$.
3. If $G/G_1 = G_2$, then

$$G = G_1 \wedge G_2, \text{ if } G_2 \text{ is a subgroup of } G,$$
$$G = G_1 \times G_2, \text{ if } G_2 \text{ is an invariant subgroup of } G.$$

4. If $G/G_1 = G_2, G/G_2 = G_1$, then $G = G_1 \times G_2$.

For example, from $S_3 = A_3 \wedge S_2$ and $S_4 = F \wedge S_3$, we have $S_3/A_3 = S_2$, and $S_4/F = S_3$ respectively.

Ex. 1.13. Show that $O_3/R_3 = Z_2$.

Chapter 2

Group Representation Theory

2.1. Linear Vector Spaces

2.1.1. Defining linear vector spaces

We assume familiarity with the usual three–dimensional vector space. We need to generalize this concept. Suppose that a set L consists of elements $\{\mathbf{x}, \mathbf{y}, \ldots\}$. The set will be called a *linear vector space* L if any element can be multiplied by a complex α or added to one another and satisfy the following conditions:

1. If $\mathbf{x}$, $\mathbf{y} \in L$, then $\mathbf{x} + \mathbf{y} \in L$.
2. $(\alpha + \beta)\mathbf{x} = \alpha\mathbf{x} + \beta\mathbf{x}$.
3. $(\alpha\beta)\mathbf{x} = \alpha(\beta\mathbf{x})$. (2-1)
4. $1\ \mathbf{x} = \mathbf{x}$.
5. $\alpha(\mathbf{x} + \mathbf{y}) = \alpha\mathbf{x} + \alpha\mathbf{y}$.
6. The set L contains a zero element (null vector), $\mathbf{0}$, such that $\mathbf{x} + \mathbf{0} = \mathbf{x}$, for all $\mathbf{x} \in L$.

The elements of $\{\mathbf{x}, \mathbf{y}, \ldots\}$ are called *vectors* of the vector space L.

For example, the set of all $n \times n$ matrices forms a linear vector space of dimension n^2. In this case the $\mathbf{x}$, $\mathbf{y}\ldots$ represent matrices and the components of $\mathbf{x}$, $\mathbf{y}$,... are the matrix elements $x_{ij}, y_{ij}, \ldots$. The components of $\alpha\mathbf{x}$ and $\mathbf{x}+\mathbf{y}$ are αx_{ij} and $x_{ij} + y_{ij}$, respectively; while the null vector is the null matrix. Later, we shall see that $\{\mathbf{x}, \mathbf{y},\ldots\}$, may represent the group elements $\{R_a, R_b, \ldots\}$.

A set of vectors is said to be *linearly dependent* if any member of the set can be written as a sum of other members of the set. Otherwise the set is *linearly independent.* In the n–dimensional space L_n, any set of n linearly independent vectors $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n\}$ form a set of basis vectors, or provide a basis (coordinate system) for L_n. Any vector $\mathbf{x}$ in L_n can be expressed as a linear combination of the basis vectors

$$\mathbf{x} = \sum_i x_i \mathbf{u}_i \ . \tag{2-2}$$

The coefficients x_i are called the coordinates of the vector $\mathbf{x}$ in the basis $\mathbf{u}_1, \ldots, \mathbf{u}_n$. In quantum mechanics the $\mathbf{u}_1, \ldots, \mathbf{u}_n$ could be the n state vectors $|\varphi_1\rangle, \ldots, |\varphi_n\rangle$, which form a complete set in L_n. Any state vector $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \sum_i a_i |\varphi_i\rangle \ . \tag{2-3}$$

In the space of $n \times n$ matrices, the basis vectors $\mathbf{u}_i$ can be chosen as the matrices $\mathbf{e}_{jk}$,

$$\mathbf{e}_{jk} = \begin{pmatrix} & \vdots & \\ \cdots & 1 & \cdots \\ & \vdots & \end{pmatrix} \begin{matrix} \\ \\ j\text{-th row} \end{matrix}, \qquad \begin{matrix} k\text{-th column} \\ \\ \\ \end{matrix} \tag{2-4}$$

where all the elements of $\mathbf{e}_{jk}$ are zero except the element at the j-th row and k-th column, which is equal to 1. Any matrix $\mathbf{x}$ is expressible in terms of the basis vectors $\mathbf{e}_{jk}$,

$$\mathbf{x} = \sum_{jk} x_{jk} \mathbf{e}_{jk} \ . \tag{2-5}$$

2.1.2 Covariant and contravariant vectors

Suppose that the coordinate system $\mathbf{u}_i$ is changed into a new coordinate system $\mathbf{u}'_i$ through a transformation $B = (b_{ij})$,

$$\mathbf{u}'_i = \sum_j b_{ij} \mathbf{u}_j \ . \tag{2-6a}$$

Under the transformation, the coordinates of a vector $\mathbf{x}$ change so that the abstract vector $\mathbf{x}$ is kept invariant:

$$\mathbf{x} = \sum_i x_i \mathbf{u}_i = \sum_i x'_i \mathbf{u}'_i \ . \tag{2-7}$$

From (2-6a) we have

$$\mathbf{u}_i = \sum_j (B^{-1})_{ij} \mathbf{u}'_j \ . \tag{2-8}$$

Substituting (2-8) into (2-7), and noting that the u'_i are linearly independent, we obtain

$$x'_j = \sum_i x_i (B^{-1})_{ij} \ .$$

Let

$$A = \tilde{B}^{-1} \ , \tag{2-9}$$

where $\sim$ represents the transposition of the matrix, so that

$$x'_i = \sum_j a_{ij} x_j \ . \tag{2-6b}$$

Let $\mathbf{u}(\mathbf{u}')$ be the column vector formed out of $\mathbf{u}_i$ $(\mathbf{u}'_i)$, and $\mathbf{x}(\mathbf{x}')$ be the column vector formed out of $x_i(x'_i)$. Equation (2-6) can now be recast as,

$$\mathbf{u}' = B\mathbf{u} \ , \tag{2-10a}$$

$$\mathbf{x}' = A\,\mathbf{x} = \tilde{B}^{-1}\mathbf{x} \ . \tag{2-10b}$$

Equations (2-10) show that the basis $\mathbf{u}$ and the coordinate vector $\mathbf{x}$ transform in different ways. We call a vector *covariant (contravariant)* if it transforms as the basis $\mathbf{u}$ (the coordinate vector $\mathbf{x}$). For an orthogonal transformation $\tilde{B} = B^{-1}$, we get $A = \tilde{B}^{-1} = B$, so that the covariant and contravariant vectors are identical.

2.1.3. The metric tensor

In quantum mechanics, the scalar product of two basis vectors $|\varphi_i\rangle$ and $|\varphi_j\rangle$ is defined as

$$(\varphi_i, \varphi_j) \equiv \langle\varphi_i|\varphi_j\rangle = \int \varphi_i^*(\mathbf{x})\varphi_j(\mathbf{x})d\mathbf{x} = g_{ij} = g_{ji}^* = \langle\varphi_j|\varphi_i\rangle^* , \tag{2-11}$$

where (g_{ij}) is a hermitian matrix known as the *metric tensor*. In quantum mechanics, we generally use an orthonormal basis for which the metric tensor components $g_{ij} = \delta_{ij}$, that is (g_{ij}) is a unit matrix.

In an n–dimensional space L_n, n orthonormal vectors form a complete set. The orthonormality is expressed as

$$\langle\varphi_i|\varphi_j\rangle = \delta_{ij} , \quad \sum_{i=1}^{n} |\varphi_i\rangle \langle\varphi_i| = 1 \tag{2-12a,b}$$

Equation (2-3) and its Hermitian conjugate can be written as

$$|\psi\rangle = \sum_i |\varphi_i\rangle\langle\varphi_i|\psi\rangle = \sum_i a_i|\varphi_i\rangle ,$$

$$\langle\psi| = \sum_i \langle\psi|\varphi_i\rangle\langle\varphi_i| = \sum_i a_i^*\langle\varphi_i| .$$

Any n linearly independent but not orthogonal vectors still form a complete set in the space L_n. However, (2-12) are replaced by the more general expressions

$$\langle\varphi_i|\varphi_j\rangle = g_{ij} \tag{2-13a}$$

$$\sum_{i,j=1}^{n} |\varphi_i\rangle(g^{-1})_{ij}\langle\varphi_j| = 1 , \tag{2-13b}$$

where g^{-1} is the inverse of the matrix (g_{ij}).

If $g_{ij} = g_i\delta_{ij}$, then $(g^{-1})_{ij} = g_i^{-1}\delta_{ij}$. Therefore, for an orthogonal but not normalized basis, we have

$$g_i^{-1}\langle\varphi_i|\varphi_j\rangle = \delta_{ij} , \tag{2-14a}$$

$$\sum_{i=1}^{n} g_i^{-1}|\varphi_i\rangle\langle\varphi_i| = 1 . \tag{2-14b}$$

An alternative way of treating the non–orthogonal basis $\{|\varphi_i\rangle\}$ is by introducing the so–called *dual basis* $\{|\overline{\varphi}_i\rangle\}$, which is orthogonal to $\{|\varphi_i\rangle\}$,

$$\langle\overline{\varphi}_i|\varphi_j\rangle = \delta_{ij} . \tag{2-15a}$$

The vectors $|\varphi_i\rangle$ and $\overline{\varphi}_i$ form what is called a *bi–orthogonal basis*. The completeness relation (2-13b) becomes

$$\sum_{i=1}^{n} |\varphi_i\rangle\langle\overline{\varphi}_i| = 1 . \tag{2-15b}$$

The above definition (2-15a) can be generalized to any linear vector space L. The scalar product is defined as

$$(\mathbf{u}_i, \mathbf{u}_j) = g_{ij} = g_{ji}^* , \tag{2-16}$$

where g_{ij} are specified complex numbers. The different specifications of the values g_{ij} correspond to different definitions of the scalar product. Once the metric tensor (g_{ij}) is given, the scalar product of any two vectors in the space L is specified

$$(\mathbf{x}, \mathbf{y}) = \Big(\sum_i x_i\mathbf{u}_i, \sum_j y_j\mathbf{u}_j\Big) = \sum_{ij} x_i^* g_{ij} y_j . \tag{2-17}$$

The scalar product is an invariant under coordinate transformations, since both $\mathbf{x}$ and $\mathbf{y}$ are invariant under coordinate transformations (see (2-7)).

A space L on which a scalar product is defined is called a *unitary space*. Different definitions of the scalar product on the same space L gives different unitary spaces. From now on we only discuss unitary spaces, and whenever we talk about basis vectors we assume that they are orthonormal unless otherwise stated. Section 2.12 is devoted to non–orthogonal bases.

2.2 Linear Operators and their Representations

If under the action of an operator R, any vector $\mathbf{x}$ in a space L changes to another vector $\mathbf{y}$ in L,

$$\mathbf{y} = R\mathbf{x} \,, \tag{2-18}$$

then the space L is said to be *closed* under the operation R, or to be an *invariant space* of the operator R. Equation (2-18) defines a mapping of the vector space onto itself. The operator R is said to be linear if

$$R(\mathbf{x}+\mathbf{z}) = R\mathbf{x} + R\mathbf{z}, \quad R(\alpha\mathbf{x}) = \alpha R\mathbf{x} \,, \tag{2-19}$$

where the action of R on $\mathbf{x}$ and $\mathbf{y}$ can be defined arbitrarily. No coordinate system is specified in the definition of the operator R, so that the operator has an intrinsic significance.

For practical applications, we always introduce a coordinate system. We employ the notation used in quantum mechanics. Let $\{|\varphi_i\rangle : i = 1, 2, \ldots, n\}$, be an orthonormal basis in a space L. Suppose that the space L is an invariant space of R; thus $R|\varphi_i\rangle$ can be expressed as a linear combination of the n basis vectors;

$$R|\varphi_i\rangle = \sum_j D_{ji}(R)|\varphi_j\rangle \,. \tag{2-20a}$$

Using the orthonormality of the basis vectors, one has

$$D_{ji}(R) = \langle\varphi_j|R|\varphi_i\rangle \,. \tag{2-21}$$

The matrix $D(R)$ is called, in the language of quantum mechanics, the *representative* of the operator R in the representation $\{\varphi_i\}$, or simply a *representation matrix*. Given $D(R)$, the action of the operator R on the basis, and in turn on any state vector $|\psi\rangle = \sum_i a_i|\varphi_i\rangle$ in L, is determined:

$$R|\psi\rangle = R\sum_i a_i|\varphi_i\rangle = \sum_i a_i R|\varphi_i\rangle = \sum_{ij} D_{ji}(R)a_i|\varphi_j\rangle \,. \tag{2-22a}$$

Here we regard the coefficients a_i constants and let the operator R act only on the basis vectors, $|\varphi_i\rangle \xrightarrow{R} |\varphi_i'\rangle$. However, the action of R on $|\psi\rangle$ can also be viewed in the following way: The basis is kept unchanged, while the coordinate of $|\psi\rangle$ (that is, in the language of quantum mechanics, the wave function of $|\psi\rangle$ in the representation $\{\varphi_i\}$) changes from $\{a_i\}$ to $\{a_i'\}$,

$$R|\psi\rangle = |\psi'\rangle = \sum_j a_j'|\varphi_j\rangle \,. \tag{2-22b}$$

Comparing (2-22a) with (2-22b), one has

$$a_j' = \sum_i D_{ji}(R)a_i \,. \tag{2-20b}$$

Equations (2-20) can be rewritten as

$$R\,|\boldsymbol{\varphi}\rangle = \tilde{D}(R)|\boldsymbol{\varphi}\rangle \,, \tag{2-23a}$$

$$R\,\mathbf{a} = \mathbf{a}' = D(R)\mathbf{a} \,, \tag{2-23b}$$

where $|\boldsymbol{\varphi}\rangle$ and $\mathbf{a}$ are column vectors. The different transformation properties of $|\boldsymbol{\varphi}\rangle$ and $\mathbf{a}$ should be compared with the covariant and contravariant transformation properties in (2-10).

Inserting RR^{-1} into Eq. (2-12a), then inserting Eq. (2-12b) into the result gives

$$\sum_j \langle\varphi_i|R|\varphi_j\rangle\langle\varphi_j|R^{-1}|\varphi_k\rangle = \delta_{ik} \ . \tag{2-24a}$$

From the definition of $D(R)$ in Eq.(2-21) we have therefore that

$$D(R^{-1}) = \big(D(R)\big)^{-1} \ . \tag{2-24b}$$

That is, the *representation of the inverse operator* R^{-1} is equal to the inverse of the representation matrix of R. Using

$$\langle\varphi_i|RS|\varphi_k\rangle = \sum_j \langle\varphi_i|R|\varphi_j\rangle\langle\varphi_j|S|\varphi_k\rangle.$$

we get

$$D(RS) = D(R)D(S) \ . \tag{2-24c}$$

For any operator R in a space L, we can define another operator $R^\dagger$ by

$$\langle\varphi_j|R^\dagger|\varphi_i\rangle \equiv \langle R\varphi_j|\varphi_i\rangle, \quad i,j = 1,2,\ldots n \ . \tag{2-25a}$$

$R^\dagger$ is called the *adjoint*, or *hermitian conjugate*, operator of R. From (2-11) and (2-25a) we have

$$D(R^\dagger) = \tilde{D}^*(R) \equiv D^\dagger(R) \ . \tag{2-25b}$$

Thus in an orthonormal basis, the representation of the adjoint operator $R^\dagger$ is the hermitian conjugate of the matrix representing the operator R.

An operator is *self-adjoint*, or hermitian, if it is identical with its adjoint:

$$R^\dagger = R \ , \tag{2-26a}$$

$$\langle\varphi_j|R|\varphi_i\rangle = \langle R\varphi_j|\varphi_i\rangle, \quad i,j = 1,2,\ldots n \ . \tag{2-26b}$$

From (2-25b), it is known that in an orthonormal basis, a hermitian operator is represented by a hermitian matrix,

$$D(R) = D^\dagger(R) \ . \tag{2-26c}$$

An operator R is said to be *unitary* if

$$\langle R\psi|R\psi'\rangle = \langle\psi|\psi'\rangle \ . \tag{2-27a}$$

Applying Eq. (2-25a) to this definition one finds that

$$\langle R\psi|R\psi'\rangle = \langle\psi|R^\dagger R|\psi'\rangle = \langle\psi|\psi'\rangle \ , \tag{2-27b}$$

so that a unitary operator satisfies

$$R^\dagger R = RR^\dagger = 1, \quad R^\dagger = R^{-1} \ . \tag{2-28a, b}$$

One can then introduce a basis and use Eqs. (2-28b), (2-25b) and (2-24b) to obtain

$$D(R^\dagger) = D(R^{-1}) \text{ and,} \tag{2-29a}$$

$$D^\dagger(R) = D^{-1}(R) \ , \tag{2-29b}$$

demonstrating that in an orthonormal basis, the representation of a unitary operator is a unitary matrix.

In summary an operator is self-adjoint or unitary if and only if Eq. (2-26a) or Eq. (2-28) respectively, holds. Those equations depend on the definition of the action of the operator in the given space and the definition of the scalar product, but are independent of the basis choice. However, the validity of Eqs. (2-26c) and (2-29) does depend on the basis choice. Those equations are only correct in an orthonormal basis. The necessary generalizations for non-orthogonal bases are given respectively by Eqs. (2-118) and (2-121a) in Sec. 2.12.

Suppose that we change basis from $|\varphi_i\rangle$ to a new one $|\varphi_i'\rangle$ through a linear transformation $B = (b_{jk})$:

$$|\varphi_j'\rangle = \sum_k b_{jk}|\varphi_k\rangle \ . \tag{2-30}$$

By applying the operator R to Eq. (2-30) one gets

$$\begin{aligned} R|\varphi_j^{'}\rangle &= \sum_k b_{jk}R|\varphi_k\rangle = \sum_{k\ell} b_{jk}D_{\ell k}(R)|\varphi_\ell\rangle \\ &= \sum_{k\ell i} b_{jk}D(R)_{\ell k}(B^{-1})_{\ell i}|\varphi_i^{'}\rangle = \sum_i D'(R)_{ij}|\varphi_i^{'}\rangle. \end{aligned} \tag{2-31a}$$

Therefore the new and old representations of R are related as

$$D^{'}(R) = \tilde{B}^{-1}D(R)\tilde{B}. \tag{2-31b}$$

For unitary transformation $B^\dagger = B^{-1}$ it becomes

$$D'(R) = AD(R)A^{-1}, \qquad A = B^* \ . \tag{2-32}$$

The above discussion applies to any linear vector space with the following modifications in notation,

$$\begin{gathered} |\varphi_i\rangle \to \mathbf{u}_i, \quad |\psi\rangle \to \mathbf{x}, \quad a_i \to x_i, \\ \langle\varphi_i|R|\varphi_j\rangle \to (\mathbf{u}_i, R\mathbf{u}_j), \quad \langle R\varphi_i|R\varphi_j\rangle \to (R\mathbf{u}_i, R\mathbf{u}_j). \end{gathered} \tag{2-33}$$

2.3. Complete Sets of Commuting Operators

2.3.1. The eigenspaces of self-adjoint operators

Consider a self-adjoint operator C in the space L_n, and suppose that

$$C|\varphi_b\rangle = \sum_a C_{ab}|\varphi_a\rangle \ , \tag{2-34a}$$

$$C_{ab} = D_{ab}(C) = \langle\varphi_a|C|\varphi_b\rangle \ . \tag{2-34b}$$

Let us find the eigenvectors $|\psi^\nu\rangle$ of C, satisfying

$$C|\psi^\nu\rangle = \nu|\psi^\nu\rangle \ . \tag{2-35a}$$

The eigenvectors can be expanded in a basis for L_n,

$$|\psi^\nu\rangle = \sum_a u_{\nu a}|\varphi_a\rangle \ . \tag{2-35b}$$

Substituting Eq. (2-35b) into (2-35a) and multiplying from the left by $\langle\varphi_a|$, we obtain

$$\sum_{b=1}^{n}(C_{ab} - \nu\delta_{ab})u_{\nu b} = 0 \ , \quad a = 1, 2, \ldots n \ . \tag{2-36}$$

The condition for the existence of non–trivial solutions to (2-36) is

$$\det|C_{ab} - \nu\delta_{ab}|_1^n = \prod_{i=1}^{k}(\nu - \nu_i)^{M_{\nu_i}} = 0 \,. \tag{2-37}$$

Equation (2-37) is called the *characteristic equation* or *expectation equation*, from which the eigenvalues ν_i along with their degeneracies M_{ν_i} can be determined. In general there are k distinct eigenvalues $\nu_1, \nu_2, \ldots, \nu_k$, with degeneracies satisfying

$$\sum_{i=1}^{k} M_{\nu_i} = n \,. \tag{2-38}$$

Substituting an eigenvalue, say ν, into Eq. (2-36), we obtain M_ν linearly independent eigenvectors,

$$|\psi_j^{(\nu)}\rangle, \quad j = 1, 2, \ldots, M_\nu \,. \tag{2-39}$$

They form an M_ν–dimensional subspace L_ν of the space L_n. The subspace L_ν is called the *eigenspace* of the operator C. Any vector in L_ν,

$$|\phi^{(\nu)}\rangle = \sum_{i=1}^{M_\nu} c_i |\psi_i^{(\nu)}\rangle \,, \tag{2-40}$$

is an eigenvector of C with the eigenvalue ν. The eigenspace can be defined symbolically by

$$CL_\nu = \nu L_\nu \,, \tag{2-41a}$$

or

$$L_\nu = \{|\psi^\nu\rangle : \quad C|\psi^\nu\rangle = \nu|\psi^\nu\rangle\} \,. \tag{2-41b}$$

Since C is self–adjoint, the eigenvectors with different eigenvalues ν are orthogonal, that is the eigenspaces L_ν are orthogonal to one another. Thus the space L_n of dimension n is decomposed into a direct sum of k orthogonal eigenspaces of C,

$$L_n = \sum_{\nu=1}^{k} \oplus L_\nu \,. \tag{2-42}$$

2.3.2 A complete set of commuting operators (CSCO)

A set of commuting operators $C = (C_1, C_2, \ldots, C_l)$ is said to be a CSCO in a space L, if in L all the eigenvalues of C are non–degenerate. Let $|\psi_\lambda\rangle$ be a simultaneous eigenvector of all operators in C. It satisfies the eigenequations

$$\begin{pmatrix} C_1 \\ \vdots \\ C_l \end{pmatrix} |\psi_{\lambda_1 \ldots \lambda_l}\rangle = \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_l \end{pmatrix} |\psi_{\lambda_1 \ldots \lambda_l}\rangle \,, \tag{2-43a}$$

which can be expressed more compactly as

$$C|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle, \quad \lambda = (\lambda_1 \ldots \lambda_l) \,, \tag{2-43b}$$

$$|\psi_\lambda\rangle = \sum_a u_{\lambda a}|\varphi_a\rangle \,. \tag{2-43c}$$

In the space L_n, C has n distinct sets of eigenvalues. Each eigenvalue λ corresponds to one eigenvector $|\psi_\lambda\rangle$. The n eigenvectors $|\psi_\lambda\rangle$ form a complete set in L_n. If all C_i are self–adjoint,

then the eigenvectors with different λ are orthogonal, so that the eigenvectors of the CSCO form a orthonormal and complete set in L_n

$$\langle\psi_\lambda|\psi_{\lambda'}\rangle = \delta_{\lambda,\lambda'}, \quad \sum_\lambda |\psi_\lambda\rangle\langle\psi_\lambda| = 1 . \tag{2-44a, b}$$

Using Eqs. (2-43c), we can re-express Eq. (2-44a, b) as

$$\sum_a u^*_{\lambda a} u_{\lambda' a} = \delta_{\lambda\lambda'}, \quad \sum_\lambda u^*_{\lambda a} u_{\lambda b} = \delta_{ab} . \tag{2-44c, d}$$

In other words, $(u_{\lambda a})$ is a unitary matrix.

It must be stressed that a CSCO is related to a particular space. A CSCO in a space L_n is in general no longer a CSCO in another space L_m.

Theorem 2.1: A CSCO for a finite dimensional vector space L can always be chosen to consist of a single operator.

Proof: We know that the basis vector $|\psi_\lambda\rangle$ for an n-dimensional vector space can always be labelled uniquely by a single discrete parameter $\lambda, \lambda = 1, 2, \ldots n$. Without loss of generality, the $|\psi_\lambda\rangle$ can be assumed to be orthonormal. Let us construct a linear operator C by

$$C = \sum_{\lambda=1}^{n} \lambda |\psi_\lambda\rangle\langle\psi_\lambda| . \tag{2-44e}$$

Obviously we have

$$C|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle . \tag{2-44f}$$

Thus each basis vector is an eigenvector of the linear operator C with the parameter λ as the eigenvalue. According to the hypothesis of the uniqueness of the label λ, the single operator C is evidently a CSCO of the space L. **QED**

The following theorem is due to Dirac (Theorem 3 in p. 78 of Dirac 1958)

Theorem 2.2 (Dirac's theorem): A linear operator that commutes with each of a complete set of commuting observables is a function of those observables.

2.4. Group Representations

A representation (rep) of a group G is a homomorphism of G onto a group $D(G)$, the elements of which are operators in a space L. If a basis is chosen for L the elements of $D(G)$ are matrices. L is called the representation space, and its dimension is called the *dimension* or *degree* of the rep $D(G)$.

If the operators are linear, $D(G)$ is said to be linear. As most reps used in physics are linear, we will deal only with linear reps in this book.

From the homomorphism we have

$$D(RS) = D(R)D(S), \quad R, S \in G , \tag{2-45a}$$

$$D(e) = I \text{ (the unit matrix)} . \tag{2-45b}$$

Hence

$$D(R^{-1}) = [D(R)]^{-1} . \tag{2-45c}$$

Ex. 2.1. If G_s is the kernel of the homomorphism $G \to D(G)$, then D(G) is a faithful representation of the factor group G/G_s.

Since state vectors in quantum mechanics are defined only up to a phase, we might deal with a group rep up to a phase. The conditions (2-45a) and (2-45c) are replaced by

$$D(RS) = \eta(R, S)D(R)D(S) , \tag{2-46a}$$

$$D(R^{-1}) = \eta^*(R, R^{-1})[D(R)]^{-1} , \tag{2-46b}$$

where $|\eta(R,S)| = 1$, and the phase factors $\eta(R,S)$ form what is known as a *factor system.* A rep satisfying (2-46a) is called a *projective* (or *ray*) rep, while a rep satisfying (2-45) is known as a *vector* rep.

Theorem 2.3: If a space L_n is an invariant subspace of G, then L_n is a representation space of G. Furthermore, if a basis $\{\varphi_i\}$ is chosen for L_n, the matrix representatives (in the usual sense used in quantum mechanics) of all the group elements in the rep space $L_n = \{\varphi_i\}$ constitute a rep D of the group G.

Proof: Since L_n is invariant under G,

$$|\varphi_i'\rangle = R_a|\varphi_i\rangle = \sum_{j=1}^{n} D_{ji}(R_a)|\varphi_j\rangle, \quad i = 1 \ldots n, \quad a = 1 \ldots g . \tag{2-47a}$$

$$D_{ji}(R_a) = \langle\varphi_j|R_a|\varphi_i\rangle . \tag{2-47b}$$

Equation (2-47a) can be put into matrix form

$$R_a\varphi = \tilde{D}(R_a)\varphi . \tag{2-48}$$

Due to (2-12a) and (2-24), the matrices defined by (2-47b) satisfy the requirement of (2-45) (for non-orthogonal bases, see Sec. 2.12). **QED**

We say that $|\varphi_i\rangle$ are the basis vectors *carrying* the rep D.

There are a few specially named reps. A rep is said to be *faithful* if the mapping $G \to D(G)$ is an isomorphism. The rep $D(R) = 1$ for all $R \in G$, is called the *identity representation.* Any abstract group has the identity rep.

The rep $D^*(G)$ which is obtained from the rep $D(G)$ by complex conjugation, is called the *conjugate representation.* If $D = D^*$ then D is called a real rep. Alternately if D and D^* are related by a similarity transformation, that is if D^* is equivalent to D (see Sec. 2.8), then D is said to be a *self-conjugate rep*

The rep $\tilde{D}^{-1}(G)$ of G is called the *contragredient rep.*

If $\{\mathbf{u}_i\}$ carry the rep $D(G)$ and $\{x_i\}$ carry the rep $\tilde{D}^{-1}(G)$, from Eqs. (2-7) and (2-10) we know that

$$\mathbf{x} = \sum_i x_i\mathbf{u}_i$$

is invariant under the group G.

For unitary reps (see Sec. 2.5),

$$\tilde{D}^{-1}(G) = D^*(G) , \tag{2-49}$$

namely, the contragredient rep is just the conjugate rep.

Theorem 2.4: If the character of a rep D is real, then D is self-conjugate.

Theorem 2.5: The character of a rep D is complex if and only if D is not self-conjugate.

Let us consider a representation for each of two groups mentioned in Chapter 1.

Example 1: The group R_2. The two orthogonal unit vectors $\mathbf{u}_1$ and $\mathbf{u}_2$ form a basis in a 2-dimensional space. The action of a rotation operator $R(\varphi)$ on the basis vectors $\mathbf{u}_i$ is defined as a rotation of $\mathbf{u}_1$ and $\mathbf{u}_2$ through angle φ

$$\begin{aligned} R(\varphi)\mathbf{u}_1 &= \mathbf{u}_1' = \cos\varphi\mathbf{u}_1 + \sin\varphi\mathbf{u}_2, \\ R(\varphi)\mathbf{u}_2 &= \mathbf{u}_2' = -\sin\varphi\mathbf{u}_1 + \cos\varphi\mathbf{u}_2 . \end{aligned} \tag{2-50}$$

From the definition (2-47), we get a 2–dimensional rep of R_2

$$D(\varphi) = D(R(\varphi)) = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} , \quad 0 \le \varphi \le 2\pi . \tag{2-51}$$

The infinite number of matrices (2-51) form a matrix group, which is a faithful rep of the group R_2.

Example 2: Representations of S_3. Suppose that there are three electrons, two in the state α (spin up) and one in the state β (spin down). The possible states in the spin space for the three electrons are

$$\begin{aligned} \varphi_1 &= x_\alpha(\xi_1)x_\alpha(\xi_2)x_\beta(\xi_3) = |\alpha\alpha\beta\rangle , \\ \varphi_2 &= x_\alpha(\xi_1)x_\beta(\xi_2)x_\alpha(\xi_3) = |\alpha\beta\alpha\rangle , \\ \varphi_3 &= x_\beta(\xi_1)x_\alpha(\xi_2)x_\alpha(\xi_3) = |\beta\alpha\alpha\rangle , \end{aligned} \tag{2-52}$$

where ξ_i is the spin coordinate of the i–th electron. The set $\{\varphi_i\}$ forms a 3–dimensional space. We define the action of an element p of the permutation group S_3 upon φ_i as a permutation of the subscripts of the spin coordinates ξ_i. For example

$$(123)|\alpha\alpha\beta\rangle = (123)\big(x_\alpha(\xi_1)x_\alpha(\xi_2)x_\beta(\xi_3)\big) = x_\alpha(\xi_2)x_\alpha(\xi_3)x_\beta(\xi_1) = |\beta\alpha\alpha\rangle . \tag{2-53}$$

In general, the operation of a cycle permutation $(jkm\ldots)$ on an n–particle product state $|i_1 i_2 \ldots i_n\rangle$ is to move the state index i_j from its original j–th place to the k–th place, and move i_k to the m–th place, etc. For example

$$(356)|i_1 i_2 i_3 i_4 i_5 i_6\rangle = |i_1 i_2 i_6 i_4 i_3 i_5\rangle .$$

Obviously, the space $\{\varphi_i\}$ is closed under the group S_3, and is a rep space of S_3. From Eq. (2-47a), it is easy to find the representative matrices:

$$\begin{matrix} D(e) \\ \begin{pmatrix} 1&0&0 \\ 0&1&0 \\ 0&0&1 \end{pmatrix} \end{matrix} \quad \begin{matrix} D(12) \\ \begin{pmatrix} 1&0&0 \\ 0&0&1 \\ 0&1&0 \end{pmatrix} \end{matrix} \quad \begin{matrix} D(13) \\ \begin{pmatrix} 0&0&1 \\ 0&1&0 \\ 1&0&0 \end{pmatrix} \end{matrix} \quad \begin{matrix} D(23) \\ \begin{pmatrix} 0&1&0 \\ 1&0&0 \\ 0&0&1 \end{pmatrix} \end{matrix} \quad \begin{matrix} D(123) \\ \begin{pmatrix} 0&1&0 \\ 0&0&1 \\ 1&0&0 \end{pmatrix} \end{matrix} \quad \begin{matrix} D(132) \\ \begin{pmatrix} 0&0&1 \\ 1&0&0 \\ 0&1&0 \end{pmatrix} \end{matrix} . \tag{2-54}$$

It should be stressed that the operation p on φ_i is defined as permuting the *subscripts of the coordinate indices* rather than the subscripts of the basis vectors. Therefore, we have (12) $\varphi_1 = \varphi_1$ rather than (12) $\varphi_1 = \varphi_2$.

Ex. 2.2. Verify that the matrices in Eq. (2-54) form a faithful rep of S_3.

Ex. 2.3. Show that the four matrices in Eq. (1-4) form a projective rep of the point group $C_{2v} = (e, C_{2z}, \sigma_x, \sigma_y)$, where σ_x and σ_y are reflection planes with normals in the x and y direction, respectively.

From the discussion above we know that the reps considered in group theory and in quantum mechanics are almost the same thing. The only differences are:

1. The rep space in quantum mechanics is always a physical space, while the rep space in group theory can be any linear vector space.
2. The operators in quantum mechanics correspond to observables and are thus always self–adjoint, while the group operators may be non self–adjoint.

We shall also see, in Sec. 2.12, that for non–orthonormal bases, the definition of the representative matrix of an operator differs between group theory and quantum mechanics.

2.5. Unitary Representations

If all the matrices of a rep are unitary,

$$D^{\dagger}(R_a) = D^{-1}(R_a) \ , \quad a = 1, 2, \ldots g \ ,$$

then the rep is called a *unitary* rep. According to Sec. 2.3, the rep of a unitary operator in an orthonormal basis must be a unitary matrix, while in a non-orthogonal basis, it can non-unitary (see Sec. 2.12.3) or unitary (see (8-87)).

If the bases $\{\varphi_i\}$ and $\{\varphi'_i\}$ are both orthonormal, then the rep $D(G)$ defined by Eq. (2-47a) is unitary. For example, the reps given by Eqs. (2-51) and (2-54) are unitary.

In Sec. 2.4, we used unit vectors as a basis for the group R_2. It is more common to use wave functions $\varphi(\mathbf{x})$ as the basis for a rep of R_2 or R_3. We define $\varphi'(\mathbf{x}) = R_z(\varphi)\varphi(\mathbf{x})$ as the new field resulting from rotating the old field $\varphi(\mathbf{x})$ through angle φ about the z-axis. Here the coordinate axes are unchanged. Under the rotation $R_z(\varphi)$, a point $P(\mathbf{x}_0)$ in the space moves to the point $P'(\mathbf{x}'_0)$ (see Fig. 2.5)

$$\mathbf{x}'_0 = R\mathbf{x}_0 \ . \tag{2-55}$$

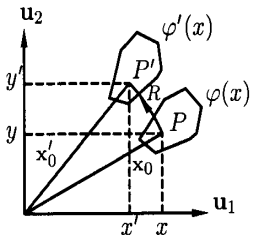


Fig. 2.5. Rotations of Points and fields.

Evidently, the value of the new field $\varphi'(\mathbf{x})$ at the new point P' is equal to the value of the old field $\varphi(\mathbf{x})$ at the original point P

$$\varphi'(\mathbf{x}'_0) = \varphi(\mathbf{x}_0) \ . \tag{2-56}$$

Inverting Eq. (2-55) one has $\mathbf{x}_0 = R^{-1}\mathbf{x}'_0$ and therefore

$$\varphi'(\mathbf{x}'_0) = \varphi(R^{-1}\mathbf{x}'_0) \ . \tag{2-57}$$

Letting $\mathbf{x}'_0 \to \mathbf{x}$ (since $\mathbf{x}'_0$ is an arbitrary point in space), one has

$$R\varphi(\mathbf{x}) = \varphi'(\mathbf{x}) = \varphi(R^{-1}\mathbf{x}) \ . \tag{2-58}$$

Operators that move the points of a space and leave the axes fixed are said to be *active.* Operators that move the axes and leave the points fixed are said to be *passive. In this book we shall use the active convention,* that is from now on we shall adhere to Eq. (2-58) as the definition for the operation of the rotation R upon a wave function $\varphi(\mathbf{x})$.

Example 1: The group R_2. Suppose that there are two points $P(x, y)$ and $P'(x', y')$ (see Fig. 2.5), and that under the rotation $R(\varphi)$, the point P goes over to P',

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = R(\varphi)\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} \ . \tag{2-59}$$

Assume that $\varphi_1(\mathbf{x})$ and $\varphi_2(\mathbf{x})$ are wave functions of a p_x electron and a p_y electron, respectively. Ignoring all irrelevant factors, $\varphi_1(\mathbf{x}) = x, \varphi_2(\mathbf{x}) = y$.

From (2-58) we have

$$\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \xrightarrow{R} \begin{pmatrix} \varphi'_1 \\ \varphi'_2 \end{pmatrix} = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \tilde{D}(\varphi)\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \ . \tag{2-60a}$$

Therefore, with $\varphi_1 = x$, and $\varphi_2 = y$ as our basis, the representation of R_2 is

$$D(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} , \tag{2-60b}$$

which is identical with (2-51). The difference between Eq. (2-59) and Eq. (2-60a) merits special attention. When x and y are regarded as coordinates, they transform according to (2-59), and if regarded as wave functions, they transform according to (2-60a). Henceforth, whenever we talk about using x, y and z as our basis, we always understand that they are wave functions instead of coordinates.

Having defined the scalar product (2-11) and the action (2-58) of group elements on $\varphi(\mathbf{x})$, we can check whether the group operator R is unitary. It is clear that

$$\langle R\varphi(\mathbf{x})|R\psi(\mathbf{x})\rangle = \int [R\varphi(\mathbf{x})]^* R\psi(\mathbf{x})d\mathbf{x} = \int \varphi^*(\mathbf{x}')\psi(\mathbf{x}')d\mathbf{x} , \tag{2-61}$$

where

$$\mathbf{x}' = R^{-1}\mathbf{x} .$$

Furthermore, the volume element is unchanged under the rotation,

$$d\mathbf{x}' = d\mathbf{x} . \tag{2-62}$$

Using this with (2-61), we have

$$\langle R\varphi(\mathbf{x})|R\psi(\mathbf{x})\rangle = \langle\varphi(\mathbf{x})|\psi(\mathbf{x})\rangle ,$$

so that the rotation operator is unitary.

In configuration space the action of other operators, such as space inversion, and plane reflection, is also defined by Eq. (2-58). Under these operations, we also have $d\mathbf{x}' = d\mathbf{x}$. Therefore, they are also unitary.

The above discussion can be easily generalized to many-particle wave functions,

$$\begin{aligned} \Psi(\mathbf{X}) &= \psi_1(\mathbf{x}_1)\psi_2(\mathbf{x}_2)\ldots\psi_n(\mathbf{x}_n), \\ \Phi(\mathbf{X}) &= \varphi_1(\mathbf{x}_1)\varphi_2(\mathbf{x}_2)\ldots\varphi_n(\mathbf{x}_n) , \\ d\mathbf{X} &= d\mathbf{x}_1 d\mathbf{x}_2 \ldots d\mathbf{x}_n = d\mathbf{X}' . \end{aligned} \tag{2-63a}$$

$$R\Psi(\mathbf{X}) = \Psi(R^{-1}\mathbf{X}) \equiv \psi_1(R^{-1}\mathbf{x}_1)\psi_2(R^{-1}\mathbf{x}_2)\ldots\psi_n(R^{-1}\mathbf{x}_n) . \tag{2-63b}$$

Consequently, these operators are still unitary in the rep space spanned by many-particle wave functions.

Example 2: Representations of $\mathcal{C}_{3v}$. Obviously (x, y, z) is a rep space of $\mathcal{C}_{3v}$. Let us find the rep of $\mathcal{C}_{3v}$ in this basis. We use $\sigma^{(\theta)}$ to designate a reflection plane, whose intersection with the xy plane has the orientation angle θ with respect to the x-axis. The three reflection planes of $\mathcal{C}_{3v}$ as shown in Fig. 1.1-2 are thus represented by

$$\sigma^{(1)} = \sigma^{120^\circ} , \quad \sigma^{(2)} = \sigma^{240^\circ} , \quad \sigma^{(3)} = \sigma^{0^\circ} = \sigma_y . \tag{2-64a}$$

For the problem here it is convenient to use cylindrical coordinates (ρ, ϕ, z). A function $\psi(\rho, \phi, z)$ under σ^θ goes over to

$$\varphi'(\rho, \phi, z) = \varphi(\rho, 2\theta - \phi, z) . \tag{2-64b}$$

Using Eqs. (2-60b) and (2-64b) the rep of $\mathcal{C}_{3v}$ can be obtained. We leave this as an exercise for the reader.

Ex. 2.4. Construct the rep of $\mathcal{C}_{3v}$ in the basis (x, y, z).

Ex. 2.5. Construct the rep of $\mathcal{C}_{4v}$ in the basis (x, y).

2.6. Regular Representation and the Group Algebra

2.6.1. Definition of the regular representation

A function Φ is said to possess *no* symmetry whatsoever with respect to a group G, if under the action of the g elements of G, it generates g linearly independent functions. A function Φ is said to be *totally symmetric* if it is invariant under G. Functions whose symmetry behavior lies between these two are said to have *partial symmetry*. For example, with respect to S_3, $|\alpha\beta\gamma\rangle, |\alpha\alpha\beta\rangle$ and $|\alpha\alpha\alpha\rangle$ are a function without symmetry, a function with partial symmetry and a totally symmetric function, respectively.

We shall always use Φ_0 to represent a function without any symmetry. For simplicity, we assume that under the action of the g elements of G, it generates g orthonormal functions

$$\varphi_a = R_a \Phi_0 \quad a = 1, 2, \ldots, g \; . \tag{2-65a}$$

$$\langle \varphi_a | \varphi_b \rangle = \delta_{ab} \; . \tag{2-65b}$$

The non–orthogonal case $\langle \varphi_a | \varphi_b \rangle = g_{ab}$ will be discussed in Sec. 3.14. The g–dimensional rep carried by $\varphi_1 \ldots, \varphi_g$ is called the *regular rep* of G

$$R_c \varphi_b = \sum_{a=1}^{g} D_{ab}(R_c) \varphi_a \; . \tag{2-66}$$

Using Eq. (2-65a), this can be rewritten as

$$R_c R_b \Phi_0 = \sum_{a=1}^{g} D_{ab}(R_c) R_a \Phi_0 \; . \tag{2-67}$$

Therefore, the matrix elements of the regular rep are given by

$$D_{ab}(R_c) = \begin{cases} 1, & \text{when} \quad R_c R_b = R_a, \\ 0, & \text{otherwise.} \end{cases} \tag{2-68}$$

The condition $R_c R_b = R_a$ is equivalent to

$$R_c R_b \Phi_0 = R_a \Phi_0, \quad \text{or} \quad R_c \varphi_b = \varphi_a \; . \tag{2-69}$$

From Eq (2-68) it is seen that in any row or any column of a matrix $D(R)$ of the regular rep, there is only one non–vanishing element (being equal to unity), and that the diagonal elements of all matrices are zeroes except for the matrix representing the identity element.

Example: The regular rep of S_3. Applying the six permutations (1-12) of S_3 to $\Phi_0 = |\alpha\beta\gamma\rangle$, we get the following six functions

$$\begin{array}{lll} \varphi_1 = e\Phi_0 \; , & \varphi_2 = (12)\Phi_0 \; , & \varphi_3 = (13)\Phi_0 \; , \\ \quad |\alpha\beta\gamma\rangle & \quad |\beta\alpha\gamma\rangle & \quad |\gamma\beta\alpha\rangle \\ \varphi_4 = (23)\Phi_0 \; , & \varphi_5 = (123)\Phi_0 \; , & \varphi_6 = (132)\Phi_0 \; . \\ \quad |\alpha\gamma\beta\rangle & \quad |\gamma\alpha\beta\rangle & \quad |\beta\gamma\alpha\rangle \end{array} \tag{2-70}$$

We can find the regular rep using definition (2-66). However the simplest way of obtaining the regular rep exploits the group table. Indeed the c–th row of Table 1.2 gives the representation matrix of the c–th element R_c of S_3,

$$\begin{array}{lll} D(e) = \{123456\} \; , & D(12) = \{216543\} \; , & D(13) = \{351624\} \; , \\ D(23) = \{465132\} \; , & D(123) = \{534261\} \; , & D(132) = \{642315\} \; , \end{array} \tag{2-71a}$$

where $\{a_1 a_2 a_3 \ldots\}$ denotes a matrix with the matrix elements all equal to one at the row a_i and column i, and zeroes elsewhere, for example

$$D(123) = \{534261\} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} . \tag{2-71b}$$

As we shall see, the regular rep plays a crucial role in the group rep theory.

2.6.2. The group space

We showed that the rows of the regular rep can be labelled by the elements of G. Thus we can regard the g elements $\{R_a\}$ of the group G, instead of the g functions $\{\varphi_a = R_a\Phi_0\}$, as the basis vectors for the regular rep. We can define the addition of R_a and the multiplication of R_a by complex numbers by the corresponding definitions for those operations on the basis vectors. (Notice that there are no such operations in the definition of the group). Thus the g elements $\{R_a\}$ form a linear vector space of dimension g, which is called the *group space*. The mapping of the group space to the space $\{\varphi_a\}$ is a one–to–one mapping. The metric tensor in the space $\{\varphi_a\}$ is defined by (2-65b), while the metric tensor for the group space can be defined in the same way:

$$\langle R_a | R_b \rangle \equiv (R_a, R_b) = g_{ab} = \delta_{ab} . \tag{2-72}$$

Any vector P in the group space is expressible in terms of the g basis vectors

$$P = \sum_{a=1}^{g} u_a R_a = \sum_{a=1}^{g} u(R_a) R_a , \tag{2-73}$$

where u_a are complex numbers. From (2-72) and (2-73) we have the scalar product of two vectors $P^{(i)}$ and $P^{(j)}$:

$$\langle P^{(i)} | P^{(j)} \rangle \equiv (P^{(i)}, P^{(j)}) = \sum_{a=1}^{g} u_a^{(i)*} u_a^{(j)} . \tag{2-74}$$

2.6.3. The group algebra

In Eq. (2-66), R_c is an operator and φ_b is a basis vector, while in the equivalent equation obtained by dividing (2-67) by Φ_0

$$R_c R_b = \sum_{a=1}^{a} D_{ab}(R_c) R_a , \tag{2-75}$$

R_c is an operator and R_b is a basis vector. To distinguish operators from basis vectors, we might put a caret above the operator, thus the previous equation becomes

$$\hat{R}_c R_b = R_c R_b = \sum_{a=1}^{g} D_{ab}(R_c) R_a . \tag{2-76}$$

This means the action of $\hat{R}_c$ upon R_b is defined by the group product $R_c R_b$. Therefore, in fact the symbol $\hat{}$ is redundant and will be omitted henceforth. However, we should keep in mind that a group element can now serves dual purposes; *it can behave as either an operator or as a basis vector.* Thus in the group space, in addition to the operation of linear combination,

$$P^{(i)} + P^{(j)} = \sum_{a} (u_a^{(i)} + u_a^{(j)}) R_a \in L_g , \tag{2-77}$$

we have another operation, multiplication according to the multiplication rule of the group. Clearly, the product of any vectors in L_g still belongs to L_g

$$P^{(i)}P^{(j)} = \sum_{ab} u_a^{(i)} u_b^{(j)} R_a R_b \in L_g \ . \tag{2-78}$$

Definition 2.1: A linear space is called an *algebra* if it is closed under a multiplication rule.

An equivalent definition follows.

Definition 2.2: A set of elements is said to form an *algebra* if the set is closed under linear combinations and multiplications.

The group space is closed under group multiplication and thus forms an algebra, called the *group algebra.* The vector P in Eq. (2-73) is called an *element* of the group algebra. If B is a subspace of A and is closed under the same multiplication rule as that of the algebra A, then B itself an algebra. The algebra B is called a *subalgebra* of the algebra A.

In analogy with the definition of the group rep $D(G)$, we can define the rep of an algebra. The representative of an element $P = \sum_a u_a R_a$ of the group algebra is defined by

$$D(P) = \sum_a u_a D(R_a) \ . \tag{2-79}$$

Thus a rep of a group gives a rep of the group algebra, and vice versa.

2.7. The Space of Functions on the Group

A vector P in the group space L_g can be expressed as (2-73), where the g complex numbers u_a, the coordinates of the vector P in the basis $\{R_a\}$, can be regarded as the components of a g–dimensional vector $\mathbf{u}$

$$\mathbf{u} = (u_1, u_2, \ldots, u_g) = (u(R_1), u(R_2), \ldots, u(R_g)) \ . \tag{2-80}$$

On the other hand, one can also regard $\mathbf{u}$ as a function $u(R)$ defined on the group manifold, in other words on the elements of the group. For discrete groups $u(R)$ is a discrete function, that is it is defined only at the g "points" $R = R_1, R_2, \ldots, R_g$. The function $u(R)$ or $u(R_a)$ is called a *function on the group* (manifold). Here the argument R or R_a should be regarded as a variable. The collection of all $\mathbf{u}$ forms a space L_F, called the *space of functions on the group.* For a finite group, there are only g independent vectors in L_F. We may choose the following g vectors as a basis of L_F

$$\mathbf{e}_1 = (1, 0, \ldots, 0), \quad \mathbf{e}_2 = (0, 1, 0, \ldots, 0), \ldots, \quad \mathbf{e}_g = (0, 0, \ldots, 1) \ . \tag{2-81}$$

The metric tensor of L_F is defined by

$$(\mathbf{e}_a, \mathbf{e}_b) = g_{ab} = \delta_{ab} \ . \tag{2-82}$$

Any vector in L_F can be expressed as

$$\mathbf{u} = \sum_{a=1}^{g} u(R_a)\mathbf{e}_a \ . \tag{2-83}$$

The scalar product of two functions on the group is thus equal to

$$\langle \mathbf{u}^{(i)} | \mathbf{u}^{(j)} \rangle = \sum_{a=1}^{g} u^{(i)}(R_a)^* u^{(j)}(R_a) \ . \tag{2-84}$$

We have already defined the operation of a group element R on a vector P in group space by (compare with Eq. (2-22a))

$$RP = R\sum_{a=1}^{g} u(R_a)R_a = \sum_{a=1}^{g} u(R_a)RR_a \ . \tag{2-85}$$

Let $RR_a = R_b$ so that $R_a = R^{-1}R_b$. Using this in (2-85) with a change in summation index from a to b gives (compare with Eq. (2-22b))

$$RP = P' = \sum_{b=1}^{g} u(R^{-1}R_b)R_b = \sum_{b=1}^{g} u'(R_b)R_b \ . \tag{2-86}$$

Therefore the operation of R on the vector P can be looked upon as changing the coordinates of P from $u(R_a)$ to $u'(R_a)$ while keeping the basis $\{R_a\}$ unchanged. We thus define the operation of group elements on functions on the group by

$$u'(R_a) = Ru(R_a) = u(R^{-1}R_a) \ . \tag{2-87a}$$

It has the same form as the operation of a rotation operator on wave functions (see (2-58)).

Notice that

$$RSu(R_a) = Ru(S^{-1}R_a) \neq u(R^{-1}S^{-1}R_a) \ .$$

Instead we have

$$RSu(R_a) = u((RS)^{-1}R_a) = u(S^{-1}R^{-1}R_a) \ . \tag{2-87b}$$

Equations (2-84) and (2-87) can be used to prove that

$$\begin{aligned}\langle R\mathbf{u}^{(i)}|R\mathbf{u}^{(j)}\rangle &= \sum_{a=1}^{g} \left(u^{(i)}(R^{-1}R_a)\right)^* u^{(j)}(R^{-1}R_a) \\ &= \sum_{b=1}^{g} \left(u^{(j)}(R_b)\right)^* u(R_b) = \langle \mathbf{u}^{(i)}|\mathbf{u}^{(j)}\rangle \ .\end{aligned}$$

Therefore, group elements are unitary operators in the space L_F.

Summarizing, there is a one–to–one correspondence between the configuration space $\{\varphi_a\}$ of (2-65a), the group space $\{R_a\}$ and the space of functions on the group, $\{u(R_a)\}$. Each of them carries the regular representation of the group G.

2.8. Equivalent Representations and Characters

If $D(G)$ and $D'(G)$ are two reps of a group G in the space L and L', respectively, and they are related by a similarity transformation

$$D'(R) = AD(R)A^{-1}, \quad R \in G \ , \tag{2-88}$$

where A is a square matrix, then we say that the reps D and D' are equivalent, and that L and L' are equivalent rep spaces. Two equivalent reps necessarily have the same dimension.

If we make the spaces L and L' identical, then (2-88) merely represents a change of basis [compare with Eq. (2-32)].

The trace of a matrix is invariant under a similarity transformation,

$$\begin{aligned}\mathrm{Tr}\, D(R)' &= \sum_i D'_{ii}(R) = \sum_{ikl} A_{ik}D_{kl}(R)A^{-1}_{li} = \sum_{kl} \delta_{kl}D_{kl}(R) \\ &= \sum_k D_{kk}(R) = \mathrm{Tr}\ D(R) \ .\end{aligned} \tag{2-89}$$

We call the trace of $D(R)$ the *character* of the element R in the rep D, and denote it by

$$\chi(R) = \text{Tr } D(R) \,. \tag{2-90}$$

Trace invariance with respect to similarity transformations implies that equivalent reps have the same set of characters. It follow from Eq. (2-90) that $\chi(e)$ is equal to the dimension of the representation.

In a manner similar to Eq. (2-89), we can use (1-17) to show that all elements of the same class have the same character. Thus the character is a function of class. We use χ_i^μ to designate the character of the i–th class in the μ–th rep.

As we said that there are an infinite number of reps of a group G which are equivalent to a given rep $D(G)$. Due to the simplicity of the unitary rep, it is most desirable to work with the unitary rep. However, not every rep of any group is equivalent to a unitary rep. Two significant types of groups do have all reps equivalent to unitary reps however.

Theorem 2.6: Any representation of a finite group is equivalent to a unitary representation.

The other type of group with all reps equivalent to unitary reps are the so–called compact Lie groups (see Sec. 5.5). We deal only with unitary reps.

Ex. 2.6. Prove that the character is a function only of the class.

2.9. Reducible and Irreducible Representations

From the two reps of $G, D^{(1)}(G)$ and $D^{(2)}(G)$, with dimensions h_1 and h_2, it is trivial to obtain a new rep D with dimension $h_1 + h_2$ by[1)]

$$D(R) = \left(\begin{array}{c|c} D^{(1)}(R) & 0 \\ \hline 0 & D^{(2)}(R) \end{array}\right) \,. \tag{2-91}$$

The rep D is called the *direct sum of the reps* $D^{(1)}$ and $D^{(2)}$, and is denoted by

$$D = D^{(1)} \oplus D^{(2)} \,. \tag{2-92}$$

The character of the rep D is

$$\chi(R) = \chi^{(1)}(R) + \chi^{(2)}(R) \,. \tag{2-93}$$

The converse to the above construction is: Given a rep $D(G)$, can we find a similarity transformation T to bring all the matrices $D(R)$ to the same block–diagonal form? If we can, then the rep D is said to be *reducible* ;[2)] otherwise, D is *irreducible* . For example, if

$$TD(R_a)T^{-1} = \left(\begin{array}{c|c} D^{(1)}(R_a) & 0 \\ \hline 0 & D^{(2)}(R_a) \end{array}\right) \,, \quad a = 1, 2 \ldots g \,, \tag{2-94}$$

then we say that the rep $D(G)$ is reduced into a direct sum of the two reps $D^{(1)}$ and $D^{(2)}$. We denote this decomposition

$$D = D^{(1)} \oplus D^{(2)}.$$

[1)] The multiplication rule for block–diagonal matrices,

$$D(R)D(S) = \left(\begin{array}{c|c} D^{(1)}(R)D^{(1)}(S) & 0 \\ \hline 0 & D^{(2)}(R)D^{(2)}(S) \end{array}\right) \,,$$

can be used to show that the $D(R)$ form a rep of G.

[2)] To be exact, what we call reducible here refers to a *fully reducible rep* (see Sec. 5.12).

An alternative definition of a reducible rep space is:

Definition 2.3: If in a rep space L we can find two subspaces $L^{(1)}$ and $L^{(2)}$, which are invariant[3] under the group G, then we say that the rep space L is *reducible* and can be reduced into a direct sum of two rep spaces

$$L = L^{(1)} \oplus L^{(2)} ,$$

otherwise, we say that the space L is *irreducible.*

A basis in an irreducible space is called *irreducible basis* . The basis vectors are denoted by ψ^{ν}_{m} or $|\nu m\rangle$, where ν is the label for the irreducible rep, and $m = 1, 2, \cdots h_{\nu}$ is the component index. The matrices with the matrix elements

$$D^{(\nu)}_{m\tilde{m}}(R) = \langle \psi^{\nu}_{m} | R | \psi^{\nu}_{\tilde{m}} \rangle, \tag{2-95}$$

are called *irreducible matrices* .

Definition 2.4: An invariant subspace of G is said to be minimal if it does not contain any non–trivial invariant subspace (that is the only invariant subspaces are the null space and the subspace itself) with respect to G.

Now we can give a more succinct definition for the irreducible space.

Definition 2.5: A minimal invariant subspace of a group G is called an irreducible space of G.

Similarly, we can define a minimal invariant subspace under an *algebra* A as the irreducible space of A and the rep generated by the irreducible space of A as the irrep *of the algebra.*

Example 1: The group R_2. Equation (2-60b) gives a 2–dimensional rep of R_2 in the basis $\varphi_1 = x$ and $\varphi_2 = y$. If we apply the following transformation (the task of finding such a transformation is a fundamental problem in group rep theory and will be discussed in great detail in the subsequent chapters) to the basis

$$\varphi'_1 = \frac{-1}{\sqrt{2}}(x + iy) = rY_{11}(\theta, \varphi), \quad \varphi'_2 = \frac{1}{\sqrt{2}}(x - iy) = rY_{1-1}(\theta, \varphi) , \tag{2-96}$$

we see that this 2–dimensional rep will be reduced into two one–dimensional reps. To show this, we compare Eq. (2-96) with Eq. (2-30), and obtain

$$B = \begin{pmatrix} -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} . \tag{2-97}$$

Using Eqs. (2-88), (2-60b) and (2-97), we obtain the rep of R_2 in the new basis (2-96) as

$$D'(\varphi) = B^{*} D(\varphi) \tilde{B} = \begin{pmatrix} e^{-i\varphi} & 0 \\ 0 & e^{i\varphi} \end{pmatrix} . \tag{2-98}$$

Ex. 2.7. Show that if the basis in (2-52) undergoes the following transformation,

$$\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} \\ \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} \\ 0 & \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}} \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{pmatrix} , \tag{2-99}$$

[3] For a fully reducible rep, we only need to find one invariant subspace $L^{(1)}$ of G, since the remaining subspace $L^{(2)}$ is necessarily invariant under G.

then the 3-dimensional rep (2-54) will be reduced.

If a rep $D(G)$ has the block-diagonal form (2-94), we shall say that $D(G)$ is in a *reduced form.* We then inquire whether or not $D^{(1)}$ and $D^{(2)}$ can be further reduced. Since each subspace can be treated independently, we discuss $D^{(1)}$ and $D^{(2)}$ separately. For example, the following transformation

$$\left(\begin{array}{c|c} T_1' & 0 \\ \hline 0 & 1 \end{array}\right) \begin{matrix} \}h_1 \\ \}h_2 \end{matrix} \tag{2-100}$$

only changes $D^{(1)}$ without affecting $D^{(2)}$. We may choose T_1' appropriately such that $D^{(1)}$ becomes block-diagonal. We continue this process until $D(G)$ becomes a direct sum of irreducible representations,

$$D(R) = \begin{pmatrix} D^{(\nu_1)}(R) & & \\ & D^{(\nu_2)}(R) & \\ & & \ddots \end{pmatrix}, \tag{2-101}$$

or

$$D(R) = \sum_i \oplus D^{(\nu_i)} = D^{(\nu_1)} \oplus D^{(\nu_2)} \oplus \dots \ . \tag{2-102}$$

Suppose that the dimensions of the rep $D(R)$ and irrep (ν_i) are h and $|\nu_i|$, respectively, then $h = \sum_i |\nu_i|$. The reducible representation space L is correspondingly decomposed into a direct sum of a number of irreducible spaces

$$L = \sum_i \oplus L_{\nu_i} = L_{\nu_1} \oplus L_{\nu_2} \oplus \dots \tag{2-103a}$$

Some of the irreps in the decomposition may be equivalent. Equivalent irreps are considered to be the same irrep. Thus, Eq. (2-102) can be rewritten as

$$D = \sum_\nu \oplus \tau_\nu D^{(\nu)} \ , \tag{2-103b}$$

where the sum runs only over the inequivalent irreps. The τ_ν are often called *multiplicities.*

The character of a reducible rep is called the *compound character,* while the character of an irreducible representation is called the *simple,* or *primitive character.* Using Eq. (2-103b), the compound character is expressible in terms of the simple characters as

$$\chi_i = \sum_\nu \tau_\nu \chi_i^{(\nu)} \ . \tag{2-103c}$$

If a rep $D(G)$ has been reduced to a form such as Eq. (2-101) where all $D^{(\nu_i)}$ are irreducible, then we say the representation $D(G)$ is in *totally reduced form.*

Since fully reducible reps (see footnote (2)) can always be reduced to a sum of irreps of lower dimensions. Therefore the problem of finding all reps of a finite group or compact Lie group is simplified to the problem of finding all the inequivalent irreps of G. A useful result that lies at the heart of our new method for solving that problem is

Theorem 2.7: If an operator C commutes with a group G, then the eigenspace L_λ of C is a representation space of G.

Proof: According to the assumption

$$[C, R_a] = 0, \quad a = 1, \dots, g \ . \tag{2-104}$$

Let $\psi^{(\lambda)}$ be a vector in the eigenspace L_λ of C,

$$C\psi^{(\lambda)} = \lambda \psi^{(\lambda)} \ . \tag{2-105a}$$

Then

$$CR_a\psi^{(\lambda)} = R_aC\psi^{(\lambda)} = \lambda R_a\psi^{(\lambda)} \ , \quad a = 1, \ldots, g \ . \tag{2-105b}$$

Therefore, $R_a\psi^{(\lambda)}$ is still an eigenvector of C with the same eigenvalue λ. It means that $R_a\psi^{\lambda} \in L_\lambda$, i.e., L_λ is an invariant subspace of G, and thus is a rep space of G. **QED**

If a rep space L of G is decomposed to a direct sum of k eigenspaces of C, $L = \sum_{i=1}^{k} \oplus L_{\lambda_i}$, then the corresponding rep D is reduced into a direct sum of k reps

$$D = \sum_{i=1}^{k} \oplus D^{(\lambda_i)}.$$

2.10. Subduced and Induced Representations

A *subduced representation* is one obtained by restricting an irrep $D^{(\nu)}$ of a group G to elements of a subgroup G_s of G, denoted by $D^{(\nu)} \downarrow G_s$. In general the subduced rep is a reducible rep of G_s, which can be reduced to a direct sum of the irreps of G_s,

$$D^{(\nu)} \downarrow G_s = \sum_{\mu} \oplus \tau_\mu^{(\nu)} D^{(\mu)}(G_s), \tag{2-106a}$$

where $\tau_\mu^{(\nu)}$ is the number of times that the irrep (μ) of G_s occurs in the subduced rep $D^{(\nu)} \downarrow G_s$.

Definition 2.6: If $\tau_\mu^{(\nu)} \leq 1$ for all possible ν and μ, then G_s is said to be a *canonical subgroup* of G.

Definition 2.7: A group chain

$$G \supset G_1 \supset G_2 \supset \ldots \supset G_n$$

is said to be a *canonical subgroup chain* if G_{i+1} is a canonical subgroup of G_i for $i = 0, 1, 2, \ldots, n-1$ with $G_0 = G$, and G_n being an Abelian group.

The above procedure for obtaining a rep of a subgroup G_s from an irrep of the larger group G is called *subduction*.

The reverse process, called *induction*, is the construction of a rep of a group G from an irrep of its subgroup G_s. The left coset decomposition of G with respect to G_s is written as

$$G = \sum_{i=1}^{q} a_i G_s \ , \tag{2-106b}$$

where a_i are coset representatives, $a_1 = e$ and $q = |G|/|G_s|$.

Let $|\mu m\rangle$ be the m-th basis vector of an irrep (μ) of G_s, with dimension h_μ. Let

$$|\mu m i\rangle \equiv a_i|\mu m\rangle \ , \quad i = 1, 2, \ldots, q \ , \quad m = 1, 2, \ldots, h_\mu \ . \tag{2-106c}$$

For any $R \in G$, Ra_i can be expressed as

$$Ra_i = a_j H \ , \quad H \in G_s \ . \tag{2-106d}$$

Thus

$$\begin{aligned} R|\mu m i\rangle &= Ra_i|\mu m\rangle = a_j H|\mu m\rangle \\ &= a_j \sum_{m'} D^{(\mu)}_{m'm}(H)|\mu m'\rangle = \sum_{m'} D^{(\mu)}_{m'm}(H)|\mu m' j\rangle \ , \end{aligned} \tag{2-106e}$$

where $D^{(\mu)}$ is the irrep of G_s. Therefore, the qh_μ vectors $|\mu mi\rangle$ are closed under the group G and thus carry a rep of G, called the *induced representation* and denoted by $D^{(\mu)} \uparrow G$, or $(\mu) \uparrow G$. The induced rep is in general reducible, so that

$$D^{(\mu)} \uparrow G = \sum_\nu \oplus \tau_\nu^{(\mu)} D^{(\nu)}(G) \tag{2-106f}$$

where $\tau_\nu^{(\mu)}$ is the number of occurrences of the irrep (ν) of G in the induced rep $(\mu) \uparrow G$.

From (2-106e) we know that the representation matrix of any element R of G in the induced rep $(\mu) \uparrow G$ is block diagonalized,

$$D^{(\mu)\uparrow G}_{kj,mi}(R) = \mathcal{G}_{ji}(R) D^{(\mu)}_{km}(a_j^{-1} R a_i) \ , \tag{2-106g}$$

where $\mathcal{G}(R)$ is called the *ground rep* of the group G with respect to the subgroup G_s,

$$\mathcal{G}_{ji}(R) = \begin{cases} 1 & \text{if } a_j^{-1} R a_i \in G_s \ , \\ 0 & \text{otherwise} \ . \end{cases} \tag{2-106h}$$

It is seen that the ground rep looks like the regular rep in that there is only one non-vanishing matrix element in each row or column. It is convenient to introduce the modified ground rep $\mathcal{D}(R)$ as

$$\mathcal{D}_{ji}(R) = \begin{cases} H \ , & \text{if } a_j^{-1} R a_i = H \in G_s \ , \\ 0 \ , & \text{otherwise} \ . \end{cases} \tag{2-106i}$$

For example, the modified ground rep of the permutation (14) of S_4 with respect to its subgroup $S_3 \times S_1$ is

$$\mathcal{D}(14) = \begin{bmatrix} 0 & 0 & 0 & (123) \\ 0 & (13) & 0 & 0 \\ 0 & 0 & (13) & 0 \\ (132) & 0 & 0 & 0 \end{bmatrix} \tag{2-106j}$$

with four coset representatives ordered as $e, (34), (234)$, and (1234).

Ex. 2.8. Find the modified ground reps of all the transpositions of S_4 with respect to its subgroup $S_3 \times S_1$.

2.11. Schur's Lemma

Schur's Lemma 1: If C is an operator commuting with a group G, and L_ν is an invariant subspace of C and an irreducible space of G, then L_ν is necessarily an eigenspace of C.

Proof: We use the method of *reduction ad absurdum*. Since L_ν is an invariant subspace of C, we can find eigenvectors of C in L_ν and gather them into eigenspaces of C. Suppose that L_ν can be decomposed into a direct sum of two eigenspaces of $C, L_\nu = L_1 \oplus L_2, CL_i = \lambda^i L_i, i = 1, 2$. Then according to Theorem 2.2, the rep space L_ν would be decomposed into a direct sum of two rep spaces of G, in contradiction with the assumption of the irreducibility of L_ν. Therefore, the only possibility is that $CL_\nu = \lambda^\nu L_\nu$. **QED**

Assume that $\psi_1^{(\nu)}, \ldots, \psi_{h_\nu}^{(\nu)}$ are the basis vectors of the irreducible space L_ν. Schur's Lemma 1 tells us

$$C\psi_i^{(\nu)} = \lambda^{(\nu)} \psi_i^{(\nu)}, \quad i = 1, 2, \ldots, h_\nu \ , \tag{2-107}$$

$$\langle \psi_i^{(\nu')} | C | \psi_j^{(\nu)} \rangle = \delta_{\nu\nu'} D_{ij}^{(\nu)}(C) = \delta_{\nu\nu'} \delta_{ij} \lambda^{(\nu)} \ . \tag{2-108}$$

Therefore, in an irreducible space L_ν of a group G, the representative of an operator which commutes with the group G and has L_ν as its invariant subspace is a multiple of the unit matrix.

Another form of Schur's Lemma 1 is

Schur's Lemma 1′: If the matrices $D(R)$ form an irrep of a group G, and if

$$AD(R) = D(R)A, \quad \text{for all } R \in G\,, \tag{2-109}$$

then A=const. I.

In other words, if a matrix commutes with all the matrices of an irrep, then the matrix is necessarily a multiple of the unit matrix.

Proof: In the irreducible space we solve the eigenequation

$$A\mathbf{x} = \lambda\mathbf{x}.$$

By Eq. (2-109), $D(R)\mathbf{x}$ is also an eigenvector of A with the same eigenvalue λ. Therefore the eigenspace of A is an invariant subspace of the group G. But this would mean that D is reducible, unless this subspace is the whole space, or the null space. The first possibility implies that A has only one eigenvalue, i.e., $A = \lambda I$, the second that $A = 0$. **QED**

Schur's Lemma plays a central role in group rep theory, since it gives the criterion for irreducibility.

Criterion for irreducibility: A rep is irreducible if and only if the only matrices which commute with all matrices of the rep are multiples of the unit matrix.

Consequently, to determine whether a rep D is irreducible, it suffices to find the matrix A from the matrix equation (2-109) and to see whether A is a multiple of the unit matrix.

It is to be noted that the converse of Schur's Lemma is not true. All we can say is that the eigenspace of an operator C which commutes with the group G is a representation space of G, which is in general reducible. In the next chapter we replace the single operator C in Theorem 2.7 with a complete set of commuting operators (CSCO), all of which commute with G, so that the common eigenspaces of the CSCO are irreducible spaces of G. Thus *the problem of finding irreps of a group G is converted into that of diagonalizing a complete set of commuting operators in the reducible representation space.*

Ex. 2.9. The group $SL(2, C)$ is represented by the set of regular 2×2 complex matrices. Show that this rep is irreducible. By applying Schur's Lemma, find the center of this group. Generalize to the case of $GL(n, C)$.

2.12. Appendix: Non–Orthogonal Bases

Although orthonormal bases are usually used, non–orthogonal bases are sometimes useful. One needs to modify a number of results for orthonormal bases before they are applicable to a non–orthogonal basis $\{|\varphi_i\rangle\}$.

2.12.1 Two definitions of the representation of an operator

(1) *Definition in group representation theory* (**GT**): Suppose that under a group G the non-orthonormal basis $|\varphi_i\rangle$ transforms as

$$R|\varphi_i\rangle = \sum_j D_{ji}(R)|\varphi_j\rangle\,. \tag{2-110a}$$

Then the matrix in (2-110a), $D(R)$, is still defined as the representative of R. However, (2-47b) is no longer true. Instead we have

$$D_{ji}(R) = \langle\overline{\varphi}_j|R|\varphi_i\rangle\,, \tag{2-110b}$$

where $|\overline{\varphi}_i\rangle$ is the dual basis defined in (2-15). From Eq. (2-15) one gets

$$|\overline{\varphi}_j\rangle = \sum_k (g^{-1})_{kj}|\varphi_k\rangle \ , \tag{2-111a}$$

$$|\varphi_k\rangle = \sum_i g_{ik}|\overline{\varphi}_i\rangle \ . \tag{2-111b}$$

Once the operation of R on $|\varphi_i\rangle$ is known we immediately get the representative $D(R)$, from Eq. (2-110a) without having to find the dual basis first, and then using (2-110b).

We now use Eq. (2-15) to prove that the rep defined by (2-110b) obeys the requirement (2-45). From $RR^{-1} = 1$, one has

$$\begin{gathered} \sum_j \langle\overline{\varphi}_i|R|\varphi_j\rangle\langle\overline{\varphi}_j|R^{-1}|\varphi_k\rangle = \langle\overline{\varphi}_i|\varphi_k\rangle = \delta_{ik} \ , \\ D(R^{-1}) = D^{-1}(R) \ . \end{gathered} \tag{2-112}$$

Furthermore,

$$\langle\overline{\varphi}_i|RS|\varphi_k\rangle = \sum_j \langle\overline{\varphi}_i|R|\varphi_j\rangle\langle\overline{\varphi}_j|S|\varphi_k\rangle \ , \tag{2-113a}$$

$$\langle\overline{\varphi}_i|e|\varphi_j\rangle = \langle\overline{\varphi}_i|\varphi_j\rangle = \delta_{ij} \ . \tag{2-113b}$$

Hence Eq. (2-45) holds.

(2) *Definition in quantum mechanics* (**QM**). The representative $\mathcal{D}(R)$ of an operator R is defined by

$$\mathcal{D}_{ji}(R) = \langle\varphi_j|R|\varphi_i\rangle \ . \tag{2-114}$$

Using Eq. (2-13b), one gets

$$\langle\varphi_i|RS|\varphi_l\rangle = \sum_{jk} \langle\varphi_i|R|\varphi_j\rangle(g^{-1})_{jk}\langle\varphi_k|S|\varphi_l\rangle \ ,$$

i.e.

$$\mathcal{D}(RS) = \mathcal{D}(R)g^{-1}\mathcal{D}(S) \ . \tag{2-115a}$$

From Eq. (2-13a) it follows that

$$\begin{gathered} \langle\varphi_i|e|\varphi_j\rangle = \langle\varphi_i|\varphi_j\rangle = g_{ij} \ , \\ \mathcal{D}(e) = g \ . \end{gathered} \tag{2-115b}$$

With $S = R^{-1}$ in (2-115a) and using (2-115b) one obtains

$$\mathcal{D}(R^{-1}) = g\mathcal{D}^{-1}(R)g \ . \tag{2-115c}$$

One sees clearly that the rep defined in quantum mechanics by Eq. (2-114) does not satisfy the group representation requirement of (2-45).

The two kinds of reps, defined by (1) and (2) of this subsection, can be related. Multiplying Eq. (2-110a) from the left by $\langle\varphi_k|$, we obtain

$$\mathcal{D}(R) = gD(R) \ . \tag{2-116}$$

2.12.2. Representations of adjoint operators

(1) In **GT**. Using Eq. (2-110) one has

$$\langle\varphi_i|R^\dagger|\varphi_k\rangle = \langle\varphi_i|\sum_j D_{jk}(R^\dagger)\varphi_j\rangle = \sum_j g_{ij}D_{jk}(R^\dagger)$$
$$= \langle R\varphi_i|\varphi_k\rangle = \langle\sum_j D_{ji}(R)\varphi_j|\varphi_k\rangle = \sum_j D^*_{ji}(R)g_{jk} \ .$$
$$D(R^\dagger) = g^{-1}\tilde{D}^*(R)g \ . \tag{2-117}$$

Hence $D(R^\dagger)) \neq D^\dagger(R) = \tilde{D}^*(R)$. Therefore, under the definition (2-110b), the representative matrix of a self-adjoint operator A is no longer hermitian. Instead, its matrix satisfies the condition

$$D(A) = g^{-1}\tilde{D}^*(A)g \ . \tag{2-118}$$

(2) In **QM**. With the definition (2-114) however, one has

$$\mathcal{D}(R^\dagger) = \mathcal{D}^\dagger(R) \equiv \tilde{\mathcal{D}}^*(R) \ . \tag{2-119}$$

Therefore, under the definition (2-114) the representative matrix of a self-adjoint operator remains hermitian for non-orthogonal bases.

2.12.3. Representations of unitary operators

(1) In **GT**. From $R^\dagger = R^{-1}$, one has

$$D(R^\dagger) = D(R^{-1}) \ , \tag{2-120a}$$

while from (2-112) and (2-117),

$$D(R^\dagger) = D(R^{-1}) = D^{-1}(R) = g^{-1}\tilde{D}^*(R)g \ . \tag{2-121a}$$

Consequently, $D^{-1}(R) \neq \tilde{D}^*(R)$, so that, $D(R)$ is in general no longer unitary, although in special cases it may be (see Eq. (8-87)).

(2) In **QM**. From $R^\dagger = R^{-1}$ one gets

$$\mathcal{D}(R^\dagger) = \mathcal{D}(R^{-1}) \ . \tag{2-120b}$$

Using Eqs. (2-119) and (2-115c), one has

$$\mathcal{D}(R^\dagger) = \mathcal{D}^\dagger(R) = \mathcal{D}(R^{-1}) = g\mathcal{D}^{-1}(R)g \ . \tag{2-121b}$$

Therefore $\mathcal{D}^\dagger(R) \neq \mathcal{D}^{-1}(R)$, i.e., $\mathcal{D}(R)$ is, in general, no longer unitary.

2.12.4. Representations under basis transformations

(1) In **GT**. If we switch to the new basis $|\varphi'_i\rangle$ given in Eq. (2-30), the corresponding new dual basis becomes

$$|\overline{\varphi}'_i\rangle = \sum_j a_{ij}|\overline{\varphi}_j\rangle \ . \tag{2-122}$$

It can then be shown that to preserve the orthonormality $\langle\overline{\varphi}'_j|\varphi'_i\rangle = \delta_{ij}$, the matrix $A = |a_{ij}|$ has to satisfy the condition

$$A = (B^\dagger)^{-1} \ . \tag{2-123a}$$

For a real B, this condition becomes

$$A = \tilde{B}^{-1} \ , \tag{2-123b}$$

This means the basis $|\varphi_i\rangle$ transforms covariantly, while the dual basis $|\overline{\varphi}_i\rangle$ transforms contravariantly. (Examples are given in Sec. 10.7).

The new representative of the operator R is

$$D'_{ji}(R) = \langle \overline{\varphi}'_j | R | \varphi'_i \rangle \ . \tag{2-124}$$

Substituting Eqs. (2-30) and (2-122) into (2-124), and using (2-123a), we get the relation

$$D'(R) = A^* D(R) \tilde{B} = \tilde{B}^{-1} D(R) \tilde{B} \ . \tag{2-125}$$

Setting $B = T^{-1}$, we obtain the familiar formula

$$D'(R) = T D(R) T^{-1} \ . \tag{2-126}$$

It is then possible to show that: (1) under a unitary transformation, an orthonormal basis goes over to another orthonormal basis; (2) the transformation between two orthonormal bases is necessarily unitary; (3) the transformation between an orthonormal basis and an non–orthogonal basis is necessarily non-unitary.

(2) In **QM**. The relation between the new and old metric tensors is

$$g'_{il} = \langle \varphi'_i | \varphi'_l \rangle = \sum_{jk} b^*_{ij} g_{jk} b_{lk} \ ,$$

which can also be written as

$$g' = B^* g \tilde{B} \ . \tag{2-127}$$

One can also show that

$$\mathcal{D}'(R) = B^* \mathcal{D}(R) \tilde{B} \ . \tag{2-128}$$

2.12.5. Eigenvectors of a self-adjoint operator

The non–orthogonal basis vectors $|\varphi_b\rangle$ can be linearly combined into eigenvectors of a self–adjoint operator C,

$$C|\psi_\lambda\rangle = \lambda |\psi_\lambda\rangle \ , \tag{2-129}$$

$$|\psi_\lambda\rangle = \sum_b u_{\lambda b} |\varphi_b\rangle \ . \tag{2-130}$$

This can be done under both definitions (2-110b) and (2-114) for the representation matrices.

(1) In **GT**. Substituting (2-130) into (2-129), then multiplying from the left by $\langle \overline{\varphi}_a |$, and making use of (2-15a) and (2-110b), one gets

$$\sum_b (D_{ab}(C) - \lambda \delta_{ab}) u_{\lambda b} = 0 \ . \tag{2-131}$$

This is the same as Eq. (2-36) for the orthonormal basis. Assuming then that C is self–adjoint,

$$\langle \psi_{\lambda'} | C | \psi_\lambda \rangle = \lambda \langle \psi_{\lambda'} | \psi_\lambda \rangle = \langle C \psi_{\lambda'} | \psi_\lambda \rangle = \lambda' \langle \psi_{\lambda'} | \psi_\lambda \rangle \ ,$$

so that

$$(\lambda - \lambda') \langle \psi_{\lambda'} | \psi_\lambda \rangle = 0 \ . \tag{2-132}$$

Therefore, the eigenvectors $|\psi_\lambda\rangle$ of C are orthogonal in λ, and can be normalized.

If C is a CSCO for the space L, then each eigenvalue λ is unique, and the orthonormality and completeness (2-44a,b) remain true. However Eqs. (2-44c,d) are not true. Substituting (2-130) into (2-44a), we get the orthonormality relation

$$\sum_{ab} u^*_{\lambda a} g_{ab} u_{\lambda' b} = \delta_{\lambda \lambda'} \ . \tag{2-133a}$$

Defining

$$v_{\lambda a} = \sum_b g_{ab} u_{\lambda b} \ , \tag{2-134}$$

we can rewrite (2-133a) as

$$\sum_a v^*_{\lambda a} u_{\lambda' a} = \delta_{\lambda\lambda'} \ . \tag{2-133b}$$

On multiplying (2-130) from the left by $\langle\varphi_a|$, one gets

$$\langle\varphi_a|\psi_\lambda\rangle = \sum_b g_{ab} u_{\lambda b} = v_{\lambda a} \ . \tag{2-135}$$

On multiplying (2-44b) from the left by $\langle\overline{\varphi}_c|$, and from the right by $|\varphi_b\rangle$, as well as using (2-130) and (2-135), one obtains the completeness,

$$\sum_\lambda v^*_{\lambda b} u_{\lambda c} = \delta_{bc} \ . \tag{2-136a}$$

Using (2-134), we may cast it in the form

$$\sum_{\lambda a} u^*_{\lambda a} g_{ab} u_{\lambda c} = \delta_{bc} \ . \tag{2-136b}$$

Finally, multiplying $|\psi_\lambda\rangle = \sum_c u_{\lambda c}|\varphi_c\rangle$ by $v^*_{\lambda b}$, summing over λ, and using (2-136a), we get the inverse of (2-130):

$$|\varphi_b\rangle = \sum_\lambda v^*_{\lambda b}|\psi_\lambda\rangle = \sum_{\lambda a} u^*_{\lambda a} g_{ab}|\psi_\lambda\rangle \ . \tag{2-137a}$$

Equation (2-136) shows that the transformation specified by the matrix $(u_{\lambda b})$, from the non-orthogonal basis $|\varphi_b\rangle$ to the orthonormal basis $|\psi_\lambda\rangle$, is not unitary.

For an orthogonal but unnormalized basis with the metric tensor $g_{ab} = g_a\delta_{ab}$, (2-136) reduces to

$$\begin{aligned} \sum_a g_a u^*_{\lambda a} u_{\lambda' a} &= \delta_{\lambda\lambda'} \ , \\ \sum_\lambda g_a u^*_{\lambda a} u_{\lambda b} &= \delta_{ab} \ , \end{aligned} \tag{2-138}$$

with the dual basis

$$|\overline{\varphi}_a\rangle = (g_a)^{-1}|\varphi_a\rangle = (\langle\varphi_a|\varphi_a\rangle)^{-1}|\varphi_a\rangle \ . \tag{2-139}$$

(2) In **QM**. Applying the operator C to (2-130), we have

$$\sum_b (C - \lambda)|\varphi_b\rangle u_{\lambda b} = 0 \ . \tag{2-140a}$$

Multiplying (2-140a) from the left by $\langle\varphi_a|$ gives

$$\sum_b \big(\mathcal{D}_{ab}(C) - \lambda g_{ab}\big) u_{\lambda b} = 0 \ , \tag{2-140b}$$

or

$$\big(\mathcal{D}(C) - \lambda g\big)\mathbf{u}_\lambda = 0 \ . \tag{2-140c}$$

Those are equivalent to the eigenequations

$$[g^{-1}\mathcal{D}(C) - \lambda\, I]\mathbf{u}_\lambda = 0 \quad \text{or} \quad [g^{-\frac{1}{2}}\mathcal{D}(C)g^{-\frac{1}{2}} - \lambda\, I]\mathbf{u}_\lambda = 0 \ . \tag{2-141}$$

According to (2-116), $g^{-1}\mathcal{D}(C) = D(C)$. Therefore, (2-141) and (2-131) describe the same result. It means that the eigenvectors of C are the same regardless of the definition for the representation matrix of C. This is what one would expect.

For an orthonormal basis, $|\overline{\varphi}_a\rangle = |\varphi_a\rangle, \mathcal{D} = D$, all the differences discussed above between the cases (1) and (2) disappear, and we are back to our previous discussion.

Henceforth we shall use the group rep theory definition (2-110b) for the representative of an operator.

Finally, one interesting point. From (2-137a), (2-111) and (2-134), one has

$$|\overline{\varphi}_a\rangle = \sum_\lambda u^*_{\lambda a}|\psi_\lambda\rangle \ . \tag{2-137b}$$

If we regard $|\varphi_a\rangle$ as an eigenvector of a non–self–adjoint operator $\mathcal{O}$ with the eigenvalue γ_a, so

$$\mathcal{O}|\varphi_a\rangle = \gamma_a|\varphi_a\rangle \ , \tag{2-142a}$$

then the dual basis $|\overline{\varphi}_a\rangle$ is an eigenvector of the adjoint operator $\mathcal{O}^\dagger$ with the eigenvalue complex conjugate to γ_a,

$$\mathcal{O}^\dagger|\overline{\varphi}_a\rangle = \gamma^*_a|\overline{\varphi}_a\rangle \ . \tag{2-142b}$$

To show this, it suffices to prove that the solutions to (2-142a, b) obey the condition $\langle\overline{\varphi}_a|\varphi_b\rangle = \delta_{ab}$,

$$\langle\overline{\varphi}_a|\mathcal{O}|\varphi_b\rangle = \gamma_b\langle\overline{\varphi}_a|\varphi_b\rangle = \langle\mathcal{O}^\dagger\overline{\varphi}_a|\varphi_b\rangle = \gamma_a\langle\overline{\varphi}_a|\varphi_b\rangle \ .$$
$$(\gamma_a - \gamma_b)\langle\overline{\varphi}_a|\varphi_b\rangle = 0.$$

Therefore, after normalization we have $\langle\overline{\varphi}_a|\varphi_b\rangle = \delta_{ab}$.

Define the column vectors

$$\mathbf{u}_\lambda = \mathrm{col}(u_{\lambda a}, u_{\lambda b}, \ldots) \ , \quad \mathbf{v}_a = \mathrm{col}(v^*_{\lambda a}, v^*_{\lambda' a}, \ldots)$$
$$\overline{\mathbf{v}}_a = \mathrm{col}(u^*_{\lambda a}, u^*_{\lambda' a}, \ldots) \ .$$

Evidently, $\mathbf{u}_\lambda$ is the representative of the eigenvector $|\psi_\lambda\rangle$ of the self–adjoint operator C in the non–orthogonal basis $\{\varphi_a\}$, while $\mathbf{v}_a(\overline{\mathbf{v}}_a)$ is the representative of the eigenvector $|\varphi_a\rangle(|\overline{\varphi_a}\rangle)$ of the non–self–adjoint operator $\mathcal{O}(\mathcal{O}^\dagger)$ in the orthonormal basis $\{\psi_\lambda\}$. Therefore, (2-133a) and (2-136b) are the orthonormality and completeness relations of $\mathbf{u}_\lambda$, while (2-133b) and (2-136a) are the "orthonormality and completeness" relations of $\mathbf{v}_a(\overline{\mathbf{v}}_a)$. In other words, (2-133) and (2-136) can be regarded either as the orthonormality and completeness relations of the eigenvectors of the self–adjoint operator C, or those of the non–self–adjoint operators $\mathcal{O}$ and $\mathcal{O}^\dagger$.

Chapter 3

Representation Theory for Finite Groups

This chapter forms the kernel of a new approach to group representation theory. Two complementary routes are suggested for studying the material. The first one simply follows the path traced out according to the sequence of topics in this book. This path follows the original steps by which the new approach to group representation theory was developed. We use the permutation group S_3, the simplest non–Abelian finite group, as a guide for establishing the general theory and show *how the question of reducing a group rep is intimately related to the elimination of degeneracy in quantum mechanics.* The second route is as follows: after reading Theorem 3.12, jump to Secs. 3.7, 3.8 and 3.9, then turn back to Theorem 3.14 in Sec. 3.3. The first route is more instructive and easily mastered by the novice, while the second one is more elegant and rigorous from the mathematical point of view. An extensive review article (Chen, Gao & Ma 1985) was written following the second route.

3.1. The Class Space and Class Operators

3.1.1. Class operators

A sum of all elements belonging to the same class is called a *class operator.* Supposing that the i–th class has g_i elements $R_1, R_2, \ldots, R_{g_i}$, the class operator C_i is

$$C_i = \sum_{l=1}^{g_i} R_l^{(i)} , \quad i = 1, 2, \ldots, N , \tag{3-1}$$

where we use $R_l^{(i)}$ to denote the l–th element of the i–th class. Sometimes we will use the so–called average class operator C^i,

$$C^i = C_i / g_i . \tag{3-2}$$

Although the group operators R are unitary, the class operators may not be. The class operators do however have the following three important properties.

(1) They commute with any element of the group G.

$$[C_i, R_a] = 0 , \quad a = 1, 2, \ldots, g . \tag{3-3}$$

Proof: According to (1-17), a conjugate operation on an element $R_l^{(i)}$ only changes it to another element $R_{l'}^{(i)}$ of the same class so

$$R_a C_i R_a^{-1} = \sum_{l=1}^{g_i} R_a R_l^{(i)} R_a^{-1} = \sum_{l'=1}^{g_i} R_{l'}^{(i)} = C_i . \tag{3-4}$$

Thus Eq. (3-3) holds. **QED**

(2) With the aid of Eqs. (3-1) and (3-3), we see that class operators also commute with each other:

$$[C_i, C_j] = 0 \ . \tag{3-5}$$

(3) Class operators are closed under group multiplication. Thus

$$C_i C_j = \sum_{k=1}^{N} C_{ij}^k C_k \ . \tag{3-6a}$$

where C_{ij}^k are integers.

Proof: According to

$$\sum_{a=1}^{g} R_a R_l^{(i)} R_a^{-1} = \sum_{a=1}^{g} R_a (R_b R_l^{(i)} R_b^{-1}) R_a^{-1} = \sum_{a=1}^{g} R_a R_{l'}^{(i)} R_a^{-1} \ ,$$

all the elements of the i–th class give the same elements in the above sum. Therefore

$$\sum_{a=1}^{g} R_a C_i R_a^{-1} = g_i \sum_{a=1}^{g} R_a R_l^{(i)} R_a^{-1} \ .$$

Applying (3-3) to this results we obtain

$$\frac{g}{g_i} C_i = \sum_{a=1}^{g} R_a R_l^{(i)} R_a^{-1} \ . \tag{3-6b}$$

On the other hand, again using (3-3), we also have

$$C_i C_j = \frac{1}{g} \sum_{a=1}^{g} R_a (C_i C_j) R_a^{-1} \ . \tag{3-6c}$$

According to (3-6b), the right–hand side of Eq. (3-6c) must consist of complete classes. Thus Eq. (3-6a) holds. **QED**

From the requirement that both sides of (3-6a) should have the same number of elements, one has

$$g_i g_j = \sum_{k=1}^{N} C_{ij}^k g_k \ . \tag{3-6e}$$

In Sec. 3.11 it will be shown that the coefficients C_{ij}^k determine the simple characters of the group G. The C_{ij}^k are called the *structure constants* of a finite group. By Eq. (3-5), we infer that C_{ij}^k is symmetric in i and j, that is,

$$C_{ij}^k = C_{ji}^k \ . \tag{3-7}$$

The three properties given above *allow the class operator to play a decisive role in the new approach to group rep theory.*

Theorem 3.1: Any operator constructed out of group operators and commuting with the group is necessarily a class operator or a linear combination of the class operators of the group.

Proof: Assume that the operator

$$A = \sum_{a=1}^{g} x_a R_a$$

commutes with the group G, where the x_a are complex numbers. This means that

$$A = R_a A R_a^{-1}, \quad a = 1, 2, \ldots, g \ .$$

Therefore,

$$A = \frac{1}{g}\sum_{a=1}^{g} R_a A R_a^{-1} = \sum_{b=1} x_b \left[\frac{1}{g}\sum_{a=1}^{g} R_a R_b R_a^{-1}\right] = \sum_{b=1}^{g} \frac{x_b}{g_b} C_b \ ,$$

where C_b is the class operator containing the element R_b. **QED**

3.1.2. The class algebra

The N-dimensional vector space spanned by the N class operators C_i of a group G is called the *class space* L_c, which is a subspace of the g-dimensional group space. Any vector Q in L_c can be expressed as a linear combination of the basis vectors C_i,

$$Q = \sum_{i=1}^{n} q_i C_i = \sum_{i=1}^{n} q(C_i) C_i \ , \tag{3-8}$$

where $q_i = q(C_i)$ are complex numbers. The sum of two vectors in L_c is defined by

$$Q^{(\nu)} + Q^{(\mu)} = \sum_{i=1}^{N} (q_i^{(\nu)} + q_i^{(\mu)}) C_i \in L_c \ . \tag{3-9}$$

Since $L_c \subset L_g$, the metric tensor g_{ij} in L_c is determined by the metric tensor in L_g. From (2-73) and (3-1a) we have

$$\langle C_i | C_j \rangle = g_{ij} = g_i \delta_{ij} \ . \tag{3-10}$$

Therefore $\{C_i\}$ is an orthogonal but not normalized basis. The scalar product of two vectors in L_c is thus equal to

$$\langle Q^{(\nu)} | Q^{(\mu)} \rangle = \sum_i g_i q_i^{(\nu)*} q_i^{(\mu)} \ . \tag{3-11}$$

Furthermore, we can use (3-6a) to define the product of two vectors in L_c as

$$Q^{(\nu)} Q^{(\mu)} = \sum_i q_i^{(\nu)} C_i \sum_j q_j^{(\mu)} C_j = \sum_{ijk} (q_i^{(\nu)} q_j^{(\mu)} C_{ij}^k) C_k \in L_c \ . \tag{3-12}$$

From (3-9) and (3-12) it is seen that the set $\{Q^{(\nu)}\}$ is closed under linear combination and group multiplication; therefore the class operators C_i form an algebra, called the *class algebra* , which is a subalgebra of the group algebra.

3.1.3. The space of functions on classes

The N complex numbers in (3-8) can be regarded either as coordinates of the vector Q in the basis $\{Q_i\}$,

$$\mathbf{q} = (q_1, q_2, \ldots, q_N) = (q(C_1), q(C_2), \ldots, q(C_N)) \ , \tag{3-13}$$

or as a *function defined on classes.* For discrete groups, it is a discrete function and only has definite values at the N "points". The collection of all $q(C_i)$ forms a space, called the *space of functions on classes.* There is a one-to-one mapping between the class space and the space of functions on classes. In analogy with Eq. (3-11), the scalar product of two vectors $\mathbf{q}^{(\nu)}$ and $\mathbf{q}^{(\mu)}$ in the space of functions on classes is defined by

$$\langle \mathbf{q}^{(\nu)} | \mathbf{q}^{(\mu)} \rangle = \sum_{i=1}^{N} g_i q^{(\nu)*}(C_i) q^{(\mu)}(C_i) \ . \tag{3-14}$$

3.1.4. The natural representation of a class algebra

In the group algebra, group elements are both operators and basis vectors, and the g group elements form the basis of the regular rep of the group. Similarly, in the class algebra, class operators are both operators and basis vectors, and the N class operators form a basis of a rep, called the *natural rep of the class algebra.* In analogy with (2-76), we have

$$\widehat{C}_i C_j = C_i C_j = \sum_k D_{kj}(C_i) C_k \ , \tag{3-15a}$$

which may be written as

$$C_i \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_N \end{pmatrix} = \tilde{D}(C_i) \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_N \end{pmatrix} . \tag{3-15b}$$

Comparing (3-15a) with (3-6a), the matrix representative of C_i in the natural rep is

$$D_{kj}(C_i) = C_{ij}^k \ . \tag{3-16}$$

Just as there is no need to distinguish between R and $\widehat{R}$, it is also unnecessary to distinguish between C_i and $\widehat{C}_i$.

Example 1: The group S_3. The three class operators of S_3 are

$$C_1 = e, \quad C_2 = (12) + (13) + (23), \quad C_3 = (123) + (132) \ . \tag{3-17}$$

From the group table of S_3, we obtain the multiplication table for the class operators of S_3.

Table 3.1. The multiplication table of the class operators of S_3.

$C_i C_j$ \ C_j	C_1	C_2	C_3
C_1	C_1	C_2	C_3
C_2	C_2	$3(C_1 + C_3)$	$2C_2$
C_3	C_3	$2C_2$	$2C_1 + C_3$

In accordance with (3-7), Table 3.1 is symmetric about the diagonal. From Eq. (3-16) and Table 3.1, we obtain the natural rep of the class operators of S_3 as

$$D(C_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \quad D(C_2) = \begin{pmatrix} 0 & 3 & 0 \\ 1 & 0 & 2 \\ 0 & 3 & 0 \end{pmatrix} , \quad D(C_3) = \begin{pmatrix} 0 & 0 & 2 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} . \tag{3-18}$$

Remark: Since the basis $\{C_i\}$ is not normalized, $D(C_2)$ and $D(C_3)$ are not hermitian, though the operators C_2 and C_3 are self-adjoint.

Example 2: The group S_4. The group S_4 has five class operators,

$$\begin{aligned} &C_1 = e, \quad C_2 = \sum_{j>i=1}^{4} (ij) \ , \quad C_3 = \sum_{k>j>i=1}^{4} [(ijk) + (ikj)] \ , \\ &C_4 = (1234) + (1243) + (1324) + (1342) + (1423) + (1432), \\ &C_5 = (12)(34) + (13)(24) + (14)(23) \ . \end{aligned} \tag{3-19}$$

The products of C_2 with the five class operators are

$$C_2\begin{pmatrix}C_1\\C_2\\C_3\\C_4\\C_5\end{pmatrix}=\begin{pmatrix}0&1&0&0&0\\6&0&3&0&2\\0&4&0&4&0\\0&0&3&0&4\\0&1&0&2&0\end{pmatrix}\begin{pmatrix}C_1\\C_2\\C_3\\C_4\\C_5\end{pmatrix}. \tag{3-20a}$$

The natural representation of C_2 is then given by

$$D(C_2)=\begin{pmatrix}0&6&0&0&0\\1&0&4&0&1\\0&3&0&3&0\\0&0&4&0&2\\0&2&0&4&0\end{pmatrix}. \tag{3-20b}$$

Example 3: The group $\mathcal{C}_{6v}$. The group $\mathcal{C}_{6v}$ is the symmetry group of a hexagon (see Fig. 3.1). It has 12 elements, six are the rotations $C_6^n = R(2n\pi/6), n = 1,2,\ldots,6$, and six are reflections about the planes $\sigma^{(1)},\ldots,\sigma^{(6)}$.

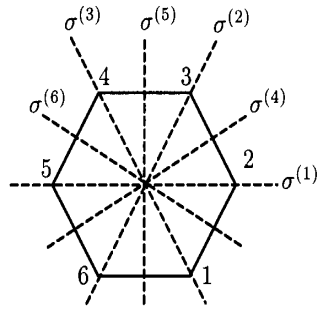


Fig. 3.1. The group $\mathcal{C}_{6v}$.

The group elements can be represented in terms of the permutations of the six vertices of the hexagon, namely,

$$\begin{array}{cccccc} e & C_6 & C_6^2 & C_6^3 & C_6^4 & C_6^5 \\ e\,, & (123456)\,, & (135)(246)\,, & (14)(25)(36)\,, & (153)(264)\,, & (165432)\,, \end{array}$$

$$\begin{array}{cccccc} \sigma^{(1)} & \sigma^{(2)} & \sigma^{(3)} & \sigma^{(4)} & \sigma^{(5)} & \sigma^{(6)} \\ (13)(46)\,, & (15)(24)\,, & (26)(35)\,, & (14)(23)(56)\,, & (16)(25)(34)\,, & (12)(36)(45)\,. \end{array} \tag{3-21}$$

Therefore, $\mathcal{C}_{6v}$ is isomorphic to a subgroup of S_6. The group $\mathcal{C}_{6v}$ has six class operators,

$$\begin{aligned} &C_1 = e\,,\ C_2 = C_6^3\,,\quad C_3 = C_6^2 + C_6^4\,,\ C_4 = C_6^1 + C_6^5\,, \\ &C_5 = \sigma^{(1)} + \sigma^{(2)} + \sigma^{(3)}\,, \qquad\qquad C_6 = \sigma^{(4)} + \sigma^{(5)} + \sigma^{(6)}\,. \end{aligned} \tag{3-22}$$

From the isomorphism (3-21), the product of group elements of $\mathcal{C}_{6v}$ can be found from the multiplication rule of the permutation group. For example, from (123456)(13)(46)=(14)(23)(56), we infer that $C_6\sigma^{(1)} = \sigma^{(4)}$. In this way we can easily write the multiplication relations for the class operators of $\mathcal{C}_{6v}$. For example,

$$C_4\begin{pmatrix}C_1\\C_2\\C_3\\C_4\\C_5\\C_6\end{pmatrix}=\begin{pmatrix}C_4\\C_3\\2C_2+C_4\\2C_1+C_3\\2C_6\\2C_5\end{pmatrix},\quad C_5\begin{pmatrix}C_1\\C_2\\C_3\\C_4\\C_5\\C_6\end{pmatrix}=\begin{pmatrix}C_5\\C_6\\2C_5\\2C_6\\3C_1+3C_3\\3C_2+3C_4\end{pmatrix}. \tag{3-23}$$

3.2. The First Kind of CSCO of G (CSCO–I)

As we indicated Theorem 2.7 is the basis of the new approach for reducing a group rep. Since each class operator commutes with the group G, it is natural to choose one of them, say C_i, as the operator C in Theorem 2.7, and decompose the representation space L of G into a direct sum of the eigenspaces L_{λ_i} of C_i, i.e.,

$$C_i L_{\lambda_i} \equiv \lambda_i L_{\lambda_i},$$
$$L = \sum_{\lambda_i} \oplus L_{\lambda_i} . \tag{3-24}$$

However, the subspace L_{λ_i} may still be reducible. We then need to choose another class operator C_j, and decompose L_{λ_i} into a direct sum of the eigenspace of C_j, so that

$$C_j L_{\lambda_i \lambda_j} = \lambda_j L_{\lambda_i \lambda_j} , \tag{3-25}$$

$$L_{\lambda_i} = \sum_{\lambda_j} \oplus L_{\lambda_i \lambda_j} , \quad L = \sum_{\lambda_i \lambda_j} \oplus L_{\lambda_i \lambda_j} . \tag{3-26}$$

Each subspace $L_{\lambda_i \lambda_j}$ is a simultaneous eigenspace of the operators C_i and C_j, and gives a representation space for G. We continue this process until each subspace cannot be further reduced by adding extra class operators of G. Now the crucial question is: How can we choose the class operators $C_i, C_j, \ldots$ so that their simultaneous eigenspaces cannot be further decomposed by adding extra class operators? Moreover, are these eigenspaces irreducible spaces of G? To address those issues, let us start with the decomposition of the class space into a direct sum of the irreducible spaces of the class algebra.

3.2.1. Reduction of the natural representation of the class algebra

The natural rep $D_{kj}(C_i) = C_{ij}^k$ is an N–dimensional reducible rep of the class algebra. Since the N class operators commute with each other, the N matrices $D(C_i), i = 1, 2, \ldots N$, can be diagonalized simultaneously. In the language of group rep theory, we have

Theorem 3.2: The natural rep D of the class algebra can be reduced to a direct sum of N one–dimensional (and thus necessarily irreducible) reps of the class algebra.

For simplicity, we first assume that all the class operators of G are self–adjoint. To reduce the natural rep, we choose one class operator, say C_{i_1}, and find its eigenvectors Q in the class space;

$$C_{i_1} Q = \lambda_{i_1} Q , \tag{3-27a}$$

$$Q = \sum_{j=1}^{N} q_j C_j . \tag{3-27b}$$

This amounts to diagonalizing the matrix $D(C_{i_1})$. From (2-36) and (3-16) we have

$$\sum_{j=1}^{N} (C_{i_1 j}^k - \lambda_{i_1} \delta_{jk}) q_j = 0, \quad k = 1, 2, \ldots, N . \tag{3-28}$$

$$\det |C_{i_1 j}^k - \lambda_{i_1} \delta_{jk}| = \prod_{\nu=1}^{n} (\lambda_{i_1} - \lambda_{i_1}^{\nu})^{M_\nu} = 0 \tag{3-29}$$

where the integer M_ν is the degeneracy of the eigenvalue $\lambda_{i_1}^{\nu}$. If there are N distinct eigenvalues, that if all the degeneracies $M_\nu = 1$, then C_{i_1} is a CSCO of the class space. Corresponding to each

eigenvalue $\lambda_{i_1}^{\nu}$, there is a unique (up to a normalization factor) solution $\mathbf{q}^{(\nu)} = (q_1^{(\nu)}, \ldots, q_N^{(\nu)})$, which in turn gives an eigenvector $Q^{(\nu)}$ of C_{i_1},

$$Q^{(\nu)} = \sum_j q_j^{(\nu)} C_j \ . \tag{3-27c}$$

According to Theorem 2.2, $Q^{(\nu)}$ is necessarily an eigenvector of all other class operators. This can also be proven in the following way. From Eqs. (3-5) and (3-27a) one has

$$C_{i_1}(C_j Q^{(\nu)}) = C_j C_{i_1} Q^{(\nu)} = \lambda_{i_1}^{\nu}(C_j Q^{(\nu)}) \ .$$

This shows that $C_j Q^{(\nu)}$ is an eigenvector of C_{i_1} with the eigenvalue $\lambda_{i_1}^{\nu}$. Since each $\lambda_{i_1}^{\nu}$ corresponds to a unique eigenvector $Q^{(\nu)}$, we have

$$C_j Q^{(\nu)} = \text{const } Q^{(\nu)} = \lambda_j^{\nu} Q^{(\nu)} \ . \tag{3-30}$$

Hence we know that the eigenvectors of the CSCO C_{i_1} are necessarily eigenvectors of all other class operators. This implies that with $Q^{(\nu)}$ as the new basis, the N class operators are all diagonalized. In the language of quantum mechanics, the non-diagonal rep of the N class operators has been transformed into the diagonal rep, that is,

$$D(C_i) = \begin{pmatrix} C_{i1}^1 & \ldots & C_{iN}^1 \\ \ldots\ldots\ldots\ldots & & \\ C_{i1}^N & \ldots & C_{iN}^N \end{pmatrix} \to \begin{pmatrix} \lambda_i^{(\nu_1)} & & & \\ & \lambda_i^{(\nu_2)} & & \\ & & \ddots & \\ & & & \lambda_i^{(\nu_N)} \end{pmatrix} \ . \tag{3-31}$$

If a certain eigenvalue, say $\lambda_{i_1}^{\mu}$, is $M_\mu(>1)$-fold degenerate, then C_{i_1} is not a CSCO of the class space. Corresponding to $\lambda_{i_1}^{\mu}$, from Eq. (3-28) we can obtain M_μ linearly independent solutions $Q_1^{(\mu)}, \ldots, Q_{M_\mu}^{(\mu)}$. They form a M_μ-dimensional eigenspace L_μ of C_{i_1}. In such a case, we can pick another class operator, say C_{i_2}, and make linear combinations of $Q_1^{(\mu)}, \ldots Q_{M_\mu}^{(\mu)}$, so that they are eigenvectors of C_{i_2} as well. We continue this process until we find a set of class operators

$$C = (C_{i_1}, C_{i_2} \ldots, C_{i_l}) \ , \tag{3-32}$$

whose simultaneous eigenspaces are all one-dimensional. C is then a CSCO of the class space. The simultaneous eigenvectors of C satisfy the following l eigenequations,

$$\begin{pmatrix} C_{i_1} \\ \vdots \\ C_{i_l} \end{pmatrix} Q^{(\nu)} = \begin{pmatrix} \lambda_{i_1}^{\nu} \\ \vdots \\ \lambda_{i_l}^{\nu} \end{pmatrix} Q^{(\nu)} \ , \tag{3-33a}$$

which can be written more succinctly as

$$C Q^{(\nu)} = \lambda^{(\nu)} Q^{(\nu)} \ , \tag{3-33b}$$

$$\lambda^{(\nu)} = (\lambda_{i_1}^{\nu}, \lambda_{i_2}^{\nu}, \ldots, \lambda_{i_l}^{\nu}) \ . \tag{3-33c}$$

3.2.2. The CSCO-I of G

Definition 3.1: If a set of operators $C = (C_{i_1}, C_{i_2}, \ldots, C_{i_l})$ selected out of the class operators is a CSCO of the class space, then C is called a CSCO of the *first kind of the group G*, or simply a CSCO of G , written as CSCO-I.

It should be emphasized that for the most commonly used finite groups, their CSCO–I consists of only one or two class operators. It is precisely this which makes our new approach to group rep theory powerful in practical calculations.

Theorem 3.3: The set of N class operators $(C_1, C_2, \ldots, C_N)$ is necessarily a CSCO of G.

Proof: We regard the diagonal matrix elements $(\lambda_i^{(\nu_1)}, \lambda_i^{(\nu_2)}, \ldots, \lambda_i^{(\nu_N)})$ in Eq. (3-31) as a column vector, and place the N column vectors together to form a matrix M,

$$M = \begin{pmatrix} \lambda_1^{(\nu_1)} & \lambda_2^{(\nu_1)} & \ldots & \lambda_N^{(\nu_1)} \\ \lambda_1^{(\nu_2)} & \lambda_2^{(\nu_2)} & \ldots & \lambda_N^{(\nu_2)} \\ \vdots & \vdots & & \vdots \\ \lambda_1^{(\nu_N)} & \lambda_2^{(\nu_N)} & \ldots & \lambda_N^{(\nu_N)} \end{pmatrix} . \tag{3-34}$$

The i–th column vector $(\lambda_i^{(\nu_1)}, \lambda_i^{(\nu_2)}, \ldots, \lambda_i^{(\nu_N)})$ is a representative of the class operator C_i. Since the N class operators are linearly independent, the N column vectors in the matrix M are also linearly independent. Therefore, the rank of the matrix M is equal to N, which in turn implies that the N row vectors $(\lambda_1^{(\nu_i)}, \lambda_2^{(\nu_i)}, \ldots, \lambda_N^{(\nu_i)})$, $i = 1, 2, \ldots, N$, are also linearly independent. Consequently, no two row vectors can be identical. Stated differently, the set of operators $(C_1, \ldots, C_N)$ has N distinct sets of eigenvalues, and thus is a CSCO of G. **QED**

It follows from Theorem 2.2 that

Theorem 3.4: Any class operator C_i of a group G is a function of the CSCO of G.

We have also Theorem 3.5.

Theorem 3.5: Any eigenvector of the CSCO of G is necessarily a simultaneous eigenvector of all the N class operators of G,

$$C_i Q^{(\nu)} = \lambda_i^{\nu} Q \ , \quad i = 1, 2, \ldots, N \ . \tag{3-33d}$$

The choice of the CSCO of G is not unique. In applications, we always want the number l of the operators which form C to be as small as possible. Therefore, we should choose such operators which have as many as possible distinct eigenvalues as the members of the CSCO. However, different CSCO's of G are equivalent in the sense that they have, according to Theorem 3.5, identical eigenvectors $Q^{(\nu)}, \nu = 1, 2, \ldots, N$. Thus we have Theorem 3.6.

Theorem 3.6: Different CSCO's of G are equivalent.

For groups whose simple characters are unknown, we can use the previous method to find the CSCO–I. For groups with known simple characters (as is the case for most finite groups), it is trivial to find their CSCO using a method to be described in Sec. 3.12. For permutation groups, we can also use formula (4-3a) to obtain their CSCO. The CSCO of the permutation groups S_2–S_6 are listed in Table 3.2-1. From Table 3.2-1 one sees that for the permutation groups S_2–S_5 only a single operator, the 2–cycle class operator, is sufficient to form a CSCO, while for S_6, two class operators are needed to form a CSCO, specifically $C = (C_{(2)}, C_{(3)})$. (For S_7, $C_{(2)}$ is the CSCO, but for S_8–S_{14}, $C = (C_{(2)}, C_{(3)})$. The results for S_7–S_{14} are not shown in Table 3.2-1).

Table 3.2-1. The new and old labelling schemes for irreps of permutation groups.

S_2	[2]
$\lambda_{(2)}$	1

S_3	[3]	[21]
$\lambda_{(2)}$	3	0

S_4	[4]	[31]	[22]
$\lambda_{(2)}$	6	2	0

S_5	[5]	[41]	[32]	[31^2]
$\lambda_{(2)}$	10	5	2	0
$\lambda_{(3)}$				

S_6	[6]	[51]	[42]	[41^2]	[33]	[321]
$\lambda_{(2)}$	15	9	5	3	3	0
$\lambda_{(3)}$				4	−8	

In Table 3.2-1 Only the positive $\lambda_{(2)}^{[\nu]}$ are listed. $\lambda_{(2)}^{[\tilde{\nu}]} = -\lambda_{(2)}^{[\nu]}$, $\lambda_{(3)}^{[\tilde{\nu}]} = \lambda_{(3)}^{[\nu]}$.

According to Theorem 2.1, the CSCO of a finite group G can always be chosen so as to consist of a single operator. If $C = (C_1, \ldots, C_l)$ is a CSCO of G, we can always find a linear combination of these l class operators so that

$$C = k_1 C_1 + \ldots + k_l C_l \tag{3-35}$$

is a CSCO of G. With known eigenvalues λ_i^ν of C_i, which are simply related to the simple characters as $\lambda_i^\nu = (g_i/h_\nu)\chi_i^\nu$ [see (3-67)], it is easy to choose the coefficients $k_1, k_2, \ldots, k_l$, so that the single operator C has N distinct eigenvalues $\lambda^\nu = \sum_{i=1}^{l} k_i \lambda_i^\nu$, and is thus a CSCO of G.

For example, for the permutation group S_6, we can choose

$$C = C_{(2)} + 3C_{(3)} \,, \tag{3-36}$$

as a CSCO, which has $N = 11$ (the number of classes of S_6) distinct eigenvalues, as listed in Table 3.2-2.

Table 3.2-2. Eigenvalues of the two kinds of CSCO-I of S_6, $(C_{(2)}, C_{(3)})$ and $(C_{(2)} + 3C_{(3)})$.

partitions / λ	[6]	[51]	[42]	[411]	[33]	[321]	[222]	[31^3]	[$2^2\,1^2$]	[21^4]	[1^6]
$\lambda_{(2)}$	15	9	5	3	3	0	−3	−3	−5	−9	−15
$\lambda_{(3)}$	40	16	0	4	−8	−5	−8	4	0	16	40
$3\lambda_{(3)}+\lambda_{(2)}$	135	57	5	15	−21	−15	−27	9	−5	39	105

In Sec. 4.5, it will be shown that for finding the irreducible basis vectors of the group S_n, we only need the $n-1$ two-cycle class operators $C_{(2)}$ of $S_n, S_{n-1}, \ldots, S_2$.

The CSCO of a group G can be understood either as a set of l class operators of (3-32), or as a single operator (3-35). Likewise, the eigenvalue $\lambda^{(\nu)}$ of C can be understood either as set of eigenvalues (3-33c), or as a single eigenvalue. However, for brevity in exposition, in proving theorems the CSCO of G is represented by a single operator C.

Theorem 3.7: An Abelian finite group G has $|G|$ one-dimensional irreps.

Proof: For an Abelian group, the group space coincides with the class space, and the irreps of the group algebra coincides with the irreps of the class algebra. The result follows from Theorem 3.2. **QED**

3.2.3. The CSCO of a direct product group $G_1 \times G_2$

Suppose that $C^{(i)}$ are the CSCO of the groups G_i with N_i classes, $i = 1, 2$. The direct product group $G_1 \times G_2$ has $N_1 N_2$ classes. The set of operators

$$C = (C^{(1)}, C^{(2)}) \tag{3-37}$$

has $N_1 N_2$ distinct sets of eigenvalues $(\lambda^{(1)}, \lambda^{(2)})$ in the class space of $G_1 \times G_2$; therefore $C = (C^{(1)}, C^{(2)})$ is the CSCO of $G_1 \times G_2$. (See Sec. 8.4.1 for examples.)

3.2.4. The case of non-self-adjoint class operators

Theorem 3.8: The CSCO of any finite group is equivalent to a self-adjoint CSCO.

Proof: Suppose that among the N class operators, n_1 are ambivalent and $2n_2$ are non-ambivalent. The non-ambivalent class operators are

$$C_i = \sum_{l=1}^{g_i} R_l^{(i)} \,, \quad C_{i'} = \sum_{l=1}^{g_i} (R_l^{(i)})^{-1} \,, \quad i = n_1 + 1, \ldots, n_1 + n_2 \,, \tag{3-38}$$

where $N = n_1 + 2n_2$. Using the unitarity of the group operators, we immediately see that the ambivalent class operators are self-adjoint, while the non-ambivalent class operators satisfy

$$C_{i'} = C_i^\dagger \ , \quad i = n_1 + 1, \ldots n_1 + n_2 \ . \tag{3-39}$$

From the $2n_2$ non-self-adjoint operators $(C_i, C_{i'})$ we can construct another $2n_2$ self-adjoint operators

$$K_j = C_l + C_{l'}, \quad K'_j = i(C_l - C_{l'}) \ , \tag{3-40}$$

$$j = l - n_1 \ , \ \ l = n_1 + 1, \ldots, n_1 + n_2 \ . \tag{3-41}$$

Thus we have a set of N self-adjoint operators

$$C' = (C_1, \ldots, C_{n_1}, \quad K_1, \ldots, K_{n_2}, \quad K'_1, \ldots, K'_{n_2}) \ .$$

The procedure used to prove Theorem 3.3 can also be used to show that C' is a CSCO of G. According to Theorem 3.6 any CSCO of G is necessarily equivalent to C'. **QED**

The significance of Theorem 3.8 is that from now on in proving theorems we can always assume that the CSCO of G is self-adjoint and utilize all the results obtained in quantum mechanics related to the self-adjoint CSCO.

For example, in the cyclic group $\{a, a^2, a^3, a^4 = e\}$ the element a has four eigenvalues, $1, i, -i$ and -1 and can be chosen as the CSCO of the group. If we choose $[(a + a^{-1}), -i(a - a^{-1})]$ as the CSCO, then all the eigenvalues are real [(2,0), (0,2), (0,−2), (0,0)]. We may also choose $2(a + a^{-1}) - i(a - a^{-1})$ as the CSCO with the eigenvalues 4, 2, −2 and 0.

Since C is equivalent to a self-adjoint CSCO, the eigenvectors of C obey the orthonormality and completeness relations

$$\langle Q^{(\nu)} | Q^{(\mu)} \rangle = \delta_{\nu\mu}, \quad \sum_\nu |Q^{(\nu)}\rangle\langle Q^{(\nu)}| = 1 \ , \tag{3-42}$$

which can be rewritten as

$$\sum_{i=1}^{N} g_i q_i^{(\nu)*} q_i^{(\mu)} = \delta_{\nu\mu} \ , \tag{3-43a}$$

$$\sum_{\nu=1}^{N} g_i q_i^{(\nu)*} q_j^{(\nu)} = \delta_{ij} \ . \tag{3-43b}$$

Notice that Eq. (3-43) has the same form as Eq. (2-138).

3.2.5. The groups S_3 and C_{6v}

Example 1: Consider the reduction of the natural rep of the class algebra of S_3. The natural rep of the S_3 class algebra is given in (3-18). Let us first diagonalize the matrix $D(C_2)$. We find three distinct eigenvalues $\lambda = 3, 0, -3$. Consequently, C_2 is a CSCO of S_3. The three associated eigenvectors are

$$\begin{aligned} \lambda = 3, \quad & Q^{(3)} = \sqrt{\tfrac{1}{6}}(C_1 + C_2 + C_3) \ , \\ \lambda = 0, \quad & Q^{(0)} = \sqrt{\tfrac{1}{6}}(2C_1 - C_3) \ , \\ \lambda = -3, \quad & Q^{(-3)} = \sqrt{\tfrac{1}{6}}(C_1 - C_2 + C_3) \ , \end{aligned} \tag{3-44a}$$

where the normalization is determined by (3-43a) with $g_1 = 1, g_2 = 3, g_3 = 2$ and the phase is decided by the requirement that $q_e^{(\nu)} > 0$ for reasons to be explained in Sec. 3.11. In the new basis $\{Q^{(3)}, Q^{(0)}, Q^{(-3)}\}$, the rep matrices of all the class operators are diagonal, specifically

$$\mathcal{D}(C_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \mathcal{D}(C_2) = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -3 \end{pmatrix}, \ \mathcal{D}(C_3) = \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} . \tag{3-44b}$$

The next example is for the dihedral group $\mathcal{C}_{6v}$. In Sec. 8.5 it will be shown that the representation problems of all the dihedral groups can be solved algebraically without solving the eigenvalue equations. Therefore the following example is given only for pedagogic purpose.

Example 2: The group $\mathcal{C}_{6v}$. From (3-23) we obtain the representative of the class operator C_4 in the natural representation,

$$D(C_4) = \left(\begin{array}{cccc|cc} 0 & 0 & 0 & 2 & & \\ 0 & 0 & 2 & 0 & & \\ 0 & 1 & 0 & 1 & \multicolumn{2}{c}{\mathbf{0}} \\ 1 & 0 & 1 & 0 & & \\ \hline & & & & 0 & 2 \\ \multicolumn{4}{c|}{\mathbf{0}} & 2 & 0 \end{array}\right) . \tag{3-45}$$

It is block-diagonal and the two submatrices can be diagonalized individually with the results

$$\begin{aligned} \lambda_4 = -1\,, \quad Q^{(-1)} &= \sqrt{\tfrac{1}{12}}(2C_1 + 2C_2 - C_3 - C_4)\,, \\ \lambda_4 = 1\,, \quad Q^{(1)} &= \sqrt{\tfrac{1}{12}}(2C_1 - 2C_2 - C_3 + C_4)\,, \end{aligned} \tag{3-46}$$

$$\lambda_4 = 2 \text{ (double root)},\ Q_1 = C_1 + C_2 + C_3 + C_4,\ Q_2 = C_5 + C_6\,, \tag{3-47}$$

$$\lambda_4 = -2 \text{ (double root)},\ Q_3 = C_1 - C_2 + C_3 - C_4,\ Q_4 = C_5 - C_6\,.$$

Due to the two-fold degeneracy of $\lambda_4 = \pm 2, C_4$ is not a CSCO of $\mathcal{C}_{6v}$. We have to choose another class operator, say C_5, and find the simultaneous eigenvectors of C_4 and C_5. For the single roots, it is easy to check that $Q^{(\pm 1)}$ are also eigenvectors of C_5 with eigenvalues zero. For the double roots, we have to solve the following eigenequations to get the eigenvectors of C_5:

$$C_5(b_1Q_1 + b_2Q_2) = \lambda_5(b_1Q_1 + b_2Q_2)\,, \quad C_5(b_3Q_3 + b_4Q_4) = \lambda_5(b_3Q_3 + b_4Q_4)\,. \tag{3-48}$$

The solutions for (λ_4, λ_5) are the following $Q^{(\lambda_4,\lambda_5)}$

$$\begin{aligned} Q^{(2,3)} &= \sqrt{\tfrac{1}{12}}(Q_1 + Q_2) = \sqrt{\tfrac{1}{12}}(C_1 + C_2 + C_3 + C_4 + C_5 + C_6), \\ Q^{(2,-3)} &= \sqrt{\tfrac{1}{12}}(Q_1 - Q_2) = \sqrt{\tfrac{1}{12}}(C_1 + C_2 + C_3 + C_4 - C_5 - C_6), \\ Q^{(-2,3)} &= \sqrt{\tfrac{1}{12}}(Q_3 + Q_4) = \sqrt{\tfrac{1}{12}}(C_1 - C_2 + C_3 - C_4 + C_5 - C_6), \\ Q^{(-2,-3)} &= \sqrt{\tfrac{1}{12}}(Q_3 - Q_4) = \sqrt{\tfrac{1}{12}}(C_1 - C_2 + C_3 - C_4 - C_5 + C_6). \end{aligned} \tag{3-49}$$

Now all degeneracies are lifted. Therefore $C = (C_4, C_5)$ is a CSCO of $\mathcal{C}_{6v}$. Consider

$$C = 2C_4 + C_5\,.$$

It has six distinct eigenvalues $\lambda = 2\lambda_4 + \lambda_5 = 7, 1, -1, -7, -4, 4$, and thus is also a CSCO of $\mathcal{C}_{6v}$.

An alternative way of finding the eigenvector $Q^{(\nu)}$ is by means of the Hamilton-Cayley theorem (Harter 1993, Sec. 1.2.B).

Ex. 3.1. Diagonalize the matrix (3-20b) and find the irreducible basis vectors $Q^{(\nu)}$ for the S_4 class algebra.

Ex. 3.2. Find the CSCO of the group $\mathcal{C}_{4v}$ and its eigenvectors in the class space.

3.3. The Projection Operator $P^{(\nu)}$

3.3.1. Decomposition of the regular rep into inequivalent reps of G

From Eqs. (3-5) and (3-27b) it follows that C and $Q^{(\nu)}$ are commutative. By (3-33b) we have

$$C(Q^{(\nu)}Q^{(\mu)}) = \begin{cases} (CQ^{(\nu)})Q^{(\mu)} = \lambda^{(\nu)}(Q^{(\nu)}Q^{(\mu)}) \\ Q^{(\nu)}(CQ^{(\mu)}) = \lambda^{(\mu)}(Q^{(\nu)}Q^{(\mu)}). \end{cases}$$

Therefore

$$Q^{(\nu)}Q^{(\mu)} = \delta_{\nu\mu}\eta_\nu Q^{(\nu)} , \tag{3-50}$$

where η_ν is a constant depending only on ν. Letting

$$P^{(\nu)} = \eta_\nu^{-1} Q^\nu , \tag{3-51}$$

we have

$$P^{(\nu)}P^{(\mu)} = \delta_{\nu\mu}P^{(\nu)} . \tag{3-52}$$

In mathematics, operators obeying Eq. (3-52) are called *idempotents.*

Using (3-43b) we invert the expansion in (3-27b) and obtain

$$C_i = \sum_{\nu=1}^{N} g_i q_i^{(\nu)*} Q^{(\nu)} . \tag{3-53}$$

Multiplying this result from the right by $Q^{(\mu)}$ and using (3-50), we have

$$\lambda_i^{(\nu)} = \eta_\nu g_i q_i^{(\nu)*} . \tag{3-54}$$

Combining (3-51), (3-53) and (3-54), we obtain

$$C_i = \sum_{\nu=1}^{N} \lambda_i^{(\nu)} P^{(\nu)} . \tag{3-55}$$

Setting $C_1 = e$, and noting that its eigenvalue is $\lambda_e^\nu = 1$, we finally get

$$e = \sum_{\nu=1}^{N} P^{(\nu)} . \tag{3-56}$$

This is the decomposition formula for the identity element of G. The implication of this formula will become more apparent as we address the group space.

Theorem 3.9: The eigenvectors $P^{(\nu)}$ of the CSCO C of G are *projection operators* onto the eigenspaces L_ν of C, and the group space can be decomposed into a direct sum of the N mutually orthogonal rep spaces L_ν.

Proof: Clearly, $P^{(\nu)}$ is an eigenvector of the CSCO of G,

$$CP^{(\nu)} = \lambda^{(\nu)}P^{(\nu)} . \tag{3-57}$$

From (3-57) we have

$$C(P^{(\nu)}R_a) = (CP^{(\nu)})R_a = \lambda^{(\nu)}(P^{(\nu)}R_a) . \tag{3-58}$$

Therefore the space

$$L_\nu \equiv P^{(\nu)}L_g \equiv \{P^{(\nu)}R_a : a = 1, 2, \ldots, g\} \tag{3-59}$$

is an eigenspace of C with the eigenvalue λ^ν. Furthermore, L_ν and L_μ are orthogonal for $\lambda^\nu \neq \lambda^\mu$. Using (3-56) we obtain

$$L_g = eL_g = \sum_{\nu=1}^{N} P^{(\nu)} L_g = \sum_{\nu=1}^{N} \oplus L_\nu \ . \tag{3-60a}$$

Thus the group space L_g is decomposed into a direct sum of N mutually orthogonal eigenspace of G, each giving a rep space of G, and $P^{(\nu)}$ is the projection operator onto the rep space L_ν. **QED**

Example: The eigenvectors $Q^{(3)}, Q^{(0)}$ and $Q^{(-3)}$ in (3-44a), which differ from $P^{(\nu)}$ by constant factors, project the group space of S_3 onto three eigenspaces of C:

One-dimensional: $L_{(3)} = e + (12) + (13) + (23) + (123) + (132)$;

One-dimensional: $L_{(-3)} = e - (12) - (13) - (23) + (123) + (132)$;

Four-dimensional: $L_{(0)}$. One can choose the basis of this eigenspace as $\{Q^{(0)}e, Q^{(0)}(12), Q^{(0)}(13), Q^{(0)}(123)\}$, that is,

$$\begin{aligned} L_{(0)} = \{&2e - (123) - (132), \quad 2(12) - (13) - (23), \\ &2(13) - (23) - (12), \quad 2(123) - (132) - e\} \ . \end{aligned}$$

Theorem 3.10: In any rep space of G, the possible eigenvalues of the CSCO of G cannot go beyond the N sets determined in the class space of G.

Proof: According to (3-56), for any rep space $\mathcal{L}$ we have

$$\mathcal{L} = e\mathcal{L} = \sum_{\nu=1}^{N} P^{(\nu)} \mathcal{L} = \sum_{\nu=1}^{N} \oplus \mathcal{L}_\nu \ . \tag{3-60b}$$

If $\mathcal{L}_\mu$ is an eigenspace of C belonging to an eigenvalue λ^μ other than those determined in the class space of G, then we must have

$$\langle \mathcal{L}_\nu | \mathcal{L}_\mu \rangle = 0 \ , \quad \text{for} \quad \nu = 1, 2, \ldots, N \ .$$

By virtue of (3-60b), this implies that

$$\langle \mathcal{L} | \mathcal{L}_\mu \rangle = 0 \ .$$

Since $\mathcal{L}$ is an arbitrary space, $\mathcal{L}_\mu$ is necessarily a null space. **QED**

Theorem 3.11: In the group space of G, the CSCO of G has N and only N distinct eigenvalues $\lambda^\nu, \nu = 1, 2, \ldots, N$, determined from the class space of G.

Proof: Since the group space contains the class space as its subspace there are at least the N distinct eigenvalues of the class space. However Theorem 3.10 implies there can be no more eigenvalues. **QED**

Theorem 3.12: The rep spaces which are eigenspaces of the CSCO of G belonging to different eigenvalues are inequivalent.

Proof: If the two representation spaces $\mathcal{L}_\nu$ and $\mathcal{L}_{\nu'}$ with different eigenvalues λ^ν and $\lambda^{\nu'}$ were equivalent, then the matrices of the CSCO of G in the two rep spaces must be related to each other by

$$D^{(\nu')}(C_i) = T D^{(\nu)}(C_i) T^{-1} \ . \tag{3-61}$$

On the other hand, since $\mathcal{L}_\nu$ and $\mathcal{L}_{\nu'}$ are eigenspaces of C, the rep of C in $\mathcal{L}_\nu(\mathcal{L}_{\nu'})$ must be equal to the unit matrix multiplied by the eigenvalue $\lambda^\nu(\lambda^{\nu'})$:

$$D^{(\nu)}(C) = \lambda^\nu \cdot I, \quad D^{(\nu')}(C) = \lambda^{\nu'} \cdot I \ . \tag{3-62}$$

Substituting Eq. (3-62) into Eq. (3-61), we get $\lambda^\nu = \lambda^{\nu'}$, contradicting the hypothesis. **QED**

Combining Theorems 3.9 and 3.12 we have

Theorem 3.9′: The group space can be decomposed into a direct sum of N inequivalent rep spaces L_ν, each being an eigenspace of the CSCO of G.

It must be emphasized that the rep space $\mathcal{L}_\nu$ is in general still *reducible*. Suppose that it can be decomposed into a direct sum of τ_ν irreducible spaces

$$\mathcal{L}_\nu = \mathcal{L}_{(\nu)1} \oplus \mathcal{L}_{(\nu)2} \oplus \ldots \oplus \mathcal{L}_{(\nu)\tau_\nu} \ . \tag{3-63}$$

Then we can show that

Theorem 3.13: The irreducible spaces $\mathcal{L}_{(\nu)k}$ with different eigenvalues λ^ν are inequivalent.

Theorem 3.14: Irreducible reps with the same eigenvalue $\lambda^{(\nu)}$ are equivalent.

A proof of this theorem is left until in Sec. 3.9.3 (see Theorem 3.24). The reader who prefers mathematical rigor to analyse of concrete problems may jump to Secs. 3.7, 3.8 and 3.9, and then turn back here.

From Theorems 3.10, 3.11, 3.13 and 3.14 we have

Theorem 3.15: A finite group G with N classes has N and only N inequivalent irreps.

Therefore, if in a space we have found an h_ν-dimensional irrep of G with the eigenvalue λ^ν, then an irrep of G in any space with the same eigenvalue λ^ν must also be of dimension h_ν.

3.3.2. Labels for irreps

From Theorems 3.13 and 3.14, we conclude that inequivalent irreps of G can be *labeled uniquely by the eigenvalue* λ^ν of the CSCO of G. In the following, we use ν to represent the eigenvalue λ^ν as well as the irrep label. One advantage of using ν as labels for the irreps is that ν is a good quantum number for a system with G as its symmetry group (see Sec. 3.20.1).

In the traditional theory on finite groups, inequivalent irreps are labelled or distinguished by the simple characters. What is the relation between these two labelling schemes? According to Theorem 3.4, any class operator of G is a function of the CSCO of G, that is

$$C_i = F_i(C) \ . \tag{3-64}$$

Therefore, the eigenvalue of C_i is a function of the eigenvalue $\lambda^{(\nu)}$ of C, so that

$$\lambda_i^{(\nu)} = F_i(\lambda^{(\nu)}) \ . \tag{3-65}$$

The relation between the eigenvalue $\lambda_i^{(\nu)}$ and the simple character of $\chi_i^{(\nu)}$ can be found as follows. From (3-1) we have

$$D^{(\nu)}(C_i) = \sum_{l=1}^{g_i} D^{(\nu)}(R_l^{(i)}) \ . \tag{3-66}$$

Since in the irrep (ν) C_i is a multiple of the unit matrix, and since elements of the same class have the same character, taking the trace of Eq. (3-66) gives

$$h_\nu \lambda_i^{(\nu)} = g_i \chi_i^{(\nu)} \ , \tag{3-67}$$

where h_ν is the dimension of the irrep (ν). Thus

$$\chi_i^{(\nu)} = \frac{h_\nu}{g_i} \lambda_i^{(\nu)} \ . \tag{3-68}$$

From (3-65) and (3-68) we get

$$\chi_i^{(\nu)} = \frac{h_\nu}{g_i} F_i(\lambda^{(\nu)}) \ . \tag{3-69}$$

This shows that the N simple characters are functions of the eigenvalue λ^ν of the CSCO of G. Therefore, the N simple characters are not functionally independent.

We use two examples to illustrate Eq. (3-64).

Example 1: The group S_3.

$$C = C_2 = \sum_{i>j=1}^{3} (ij) \ , \quad C_3 = \frac{1}{3}(C)^3 - e \ . \tag{3-70}$$

Example 2: The group S_4.

$$C = C_2 = \sum_{i>j=1}^{4} (ij) \ , \quad C_3 = -\frac{1}{48}(C)^4 + \frac{13}{12}(C)^2 - 4e \ . \tag{3-71}$$

$$C_4 = \frac{1}{16}(C)^3 - \frac{5}{4}(C)^2 \ , \quad C_5 = \frac{1}{32}(C)^4 - \frac{9}{8}(C)^2 + 3e \ . \tag{3-72}$$

3.3.3. Decomposition of an arbitrary rep space

According to Theorem 3.14, reps generated by the irreducible spaces $\mathcal{L}_{(\nu)k}$ in (3-63) are all equivalent and labelled by the same irrep label (ν). Therefore, if a function $\psi^{(\nu)}$ belongs to the eigenspace $\mathcal{L}_\nu$ of C, then $\psi^{(\nu)}$ is necessarily a basis vector for one of those equivalent irreps, or a linear combination of their basis vectors. This leads to Definition 3.2.

Definition 3.2: If a vector $\psi^{(\nu)}$ belongs to the eigenspace $\mathcal{L}_\nu$ of the CSCO of G, the $\psi^{(\nu)}$ is said to belong to the irrep (ν) of G.

Remark: Since the eigenspace $\mathcal{L}_\nu$ is in general reducible, if both $\psi_1^{(\nu)}$ and $\psi_2^{(\nu)}$ belong to the irrep (ν), it does not necessarily mean that they belong to the same irreducible space. For example, $\psi_1^{(\nu)}$ may belong to the first irreducible space $\mathcal{L}_{(\nu)1}$, while $\psi_2^{(\nu)}$ may belong to the second irreducible space $\mathcal{L}_{(\nu)2}$.

Theorem 3.16: A sufficient and necessary condition for a function $\psi^{(\nu)}$ to belong to the irrep (ν) of a group G is that $\psi^{(\nu)}$ be an eigenfunction of the CSCO of G, that is,

$$C\psi^{(\nu)} = \nu\psi^{(\nu)} \ . \tag{3-73}$$

Proof: Suppose $\psi^{(\nu)}$ is a vector in an irreducible space L of G. Obviously L is a rep space for any class operator of G and thus is an invariant subspace of C. According to Schur's Lemma 1, $\psi^{(\nu)}$ is necessarily an eigenfunction of C.

The sufficiency follows trivially from Definition 3.2. **QED**

Theorem 3.16 is the corner stone of the eigenfunction method (EFM) for group representations. It converts the problem of finding irreps of a group G into that of finding the eigenfunctions of the CSCO of G, or equivalently of diagonalizing the representative of the CSCO of G in the reducible basis $\varphi_1, \ldots, \varphi_n$. Let

$$\psi^{(\nu)} = \sum_{i=1}^{n} a_i \varphi_i \tag{3-74}$$

be the sought after eigenfunctions of C. The eigenvalue of ν and coefficients a_i are to be determined by

$$\begin{pmatrix} C_{11} & C_{12} & \ldots & C_{1n} \\ C_{21} & C_{22} & \ldots & C_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ C_{n1} & C_{n2} & \ldots & C_{nn} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} = \nu \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \ , \tag{3-75a}$$

where

$$C_{ij} = \langle \varphi_i | C | \varphi_j \rangle \ . \tag{3-76a}$$

For the majority of point groups and for all permutation groups, C is self-adjoint and the C_{ij} are real. In such cases, (C_{ij}) is a real and symmetric matrix,

$$C_{ij} = C_{ji} \ . \tag{3-76b}$$

From (3-75a) and (3-76a) we obtain

$$\sum_j \langle \varphi_j | C | \varphi_i \rangle a_j = \nu a_i . \tag{3-75b}$$

The last result is very useful. It shows that in order to obtain an equation for the variable a_i, one needs only to know the action of C on the state $|\varphi_i\rangle$.

A natural extension of Theorem 3.16 is Theorem 3.17 .

Theorem 3.17: A necessary and sufficient condition for $\psi^{(\nu)}_{\lambda(s_1),\lambda(s_2),\ldots}$ to belong to the irreps $\nu, \lambda(s_1), \lambda(s_2), \ldots$ of a subgroup chain $G \supset G(s_1) \supset G(s_2) \supset \ldots$ is that it satisfies the following eigenequations:

$$\begin{pmatrix} C \\ C(s_1) \\ C(s_2) \\ \vdots \end{pmatrix} \psi^{(\nu)}_{\lambda(s_1),\lambda(s_2),\ldots} = \begin{pmatrix} \nu \\ \lambda(s_1) \\ \lambda(s_2) \\ \vdots \end{pmatrix} \psi^{(\nu)}_{\lambda(s_1),\lambda(s_2),\ldots} , \tag{3-77a}$$

where $C(s_i)$ is the CSCO of $G(s_i)$.

Usually there is more than one value of $\lambda(s_1)$ that goes with the same quantum number ν, since the irrep of G is reducible in restricting to its subgroup $G(s_1)$,

$$D^{(\nu)} \downarrow G(s_1) = \sum_i \oplus \tau_i^{(\nu)} D^{\lambda^i(s_1)}\big(G(s_1)\big) \ .$$

If $G(s_1)$ is a *canonical subgroup* of G, then $\tau_i^{(\nu)} \leq 1$. The same applies to the relation between $\lambda(s_1)$ and $\lambda(s_2)$, and so on.

For simplicity, we use $G(s)$ to denote the chain of subgroups $G(s_1) \supset G(s_2) \supset \ldots, C(s)$ the set of operators $\big(C(s_1), C(s_2), \ldots,\big)$ and m the set of eigenvalues $\big(\lambda(s_1), \lambda(s_2), \ldots\big)$. The set of operators $C(s)$ will be referred to as the *CSCO of the subgroup chain* $G(s)$.

Theorem 3.17 can then be written as

Theorem 3.17': A necessary and sufficient condition for $\psi^{(\nu)}_m$ to belong to the irrep (ν, m) of the subgroup chain $G \supset G(s)$ is that $\psi^{(\nu)}_m$ satisfies the eigenequations

$$\begin{pmatrix} C \\ C(s) \end{pmatrix} \psi^{(\nu)}_m = \begin{pmatrix} \nu \\ m \end{pmatrix} \psi^{(\nu)}_m \ . \tag{3-77b}$$

The basis $\psi^{(\nu)}_m$ is referred to as the $G \supset G(s)$ *irreducible basis* .

Suppose that the eigenspace $\mathcal{L}_\nu = \{\psi^{(\nu)} : C\psi^{(\nu)} = \nu\psi^{(\nu)}\}$ is an irreducible space of G. Then the degeneracy M_ν of the eigenvalue ν in Eq. (3-75a) is equal to the dimension of the irrep $(\nu), M_\nu = h_\nu$. If $G \supset G(s)$ is a canonical subgroup chain we know, from the discussion following (3-77a), that this degeneracy can be totally lifted by the eigenequations of $C(s)$. That is the degeneracies for the sets of eigenvalues (ν, m_i) are all equal to unity for $i = 1, 2, \ldots h_\nu$. (Note that the degeneracies of (ν, m_i) must be independent of i, since if $\mathcal{L}_\nu$ contains the irrep (ν) τ_ν times, then each component m has to occur τ_ν times.)

Conversely, if we can find a subgroup chain $G \supset G(s)$, such that the set of the eigenvalues (ν, m) of $(C, C(s))$ is non–degenerate, then $G \supset G(s)$ is a *canonical subgroup chain* , and $\mathcal{L}_\nu$

is irreducible. Corresponding to each $(\nu, m), m = m_1, \ldots, m_{h_\nu}$, there is only one eigenvector. These h_ν eigenvectors $\psi_m^{(\nu)}$ carry an irrep of G. Therefore, for such cases the irreducible basis for $G \supset G(s)$ can be found from Eq. (3-77b) without any knowledge of the characters or irreducible matrices.

With a known irreducible basis, we can use (2-20a) or (2-21) to find the irreducible matrices.

Suppose now that $\mathcal{L}_\nu$ is reducible as shown in (3-63), and $G \supset G(s)$ is a canonical subgroup chain. Then the degeneracy M_ν of ν in Eq. (3-75a) is equal to $M_\nu = \tau_\nu h_\nu$, while the degeneracy of (ν, m) is equal to the multiplicity τ_ν. For a given (ν, m), from Eq. (3-77b) we can find τ_ν linearly independent eigenvectors $\psi_m^{(\nu)\tau}, \tau = 1, 2, \ldots, \tau_\nu$, which can be chosen as orthogonal in the *multiplicity label* τ.

Remark: Since here the multiplicity indices τ are chosen independently for each component index m, in general $\psi_m^{(\nu)\tau}$ and $\psi_{m'}^{(\nu)\tau}$ do not belong to the same irreducible space. The problem of how to find the irreducible basis for such cases is relegated to Sec. 3.13.

3.4. The Reduction of the Representations of $\mathcal{C}_{3v}$, $\mathbf{S}_2$ and $\mathbf{S}_3$

3.4.1. The group $\mathcal{C}_{3v}$

We begin with the simple problem of finding an irreducible basis for the point group $\mathcal{C}_{3v}$ using the polynomials of degree one and two in x, y and z. Using the notation of Eq. (2-64a), the CSCO of $\mathcal{C}_{3v}$ is $C = \sigma^{0^\circ} + \sigma^{120^\circ} + \sigma^{60^\circ}$.

To find the irreducible bases, we solve the eigenequation (3-73). Using (2-64b) we immediately have

$$\begin{aligned} &Cz = 3z, \\ &C \exp(i\varphi) = \exp(-i\varphi) + \exp[i(240^\circ - \varphi)] + \exp[i(120^\circ - \varphi)] = 0\ , \\ &C \exp(-i\varphi) = 0\ . \end{aligned}$$

Here the eigenvalue 3 is a single root, and the corresponding eigenspace $\mathcal{L}_{(3)}, \{z\}$, is one–dimensional and thus irreducible. The irrep (3) of $\mathcal{C}_{3v}$ is the identity rep. On the other hand the eigenvalue 0 is a double root, and $\mathcal{L}_{(0)} = (e^{i\varphi}, e^{-i\varphi})$ carries a two–dimensional rep of $\mathcal{C}_{3v}$. Let us try to lift the degeneracy by finding the eigenvectors of the CSCO of a subgroup, say $\mathcal{C}_{sy} = (e, \sigma^{0^\circ})$, of $\mathcal{C}_{3v}$. Now $C(s) = \sigma^{0^\circ} = \sigma_y$, and its eigenvectors are x and y corresponding to the eigenvalues 1 and -1. Therefore $(\nu, m) = (0, \pm 1)$, has no degeneracy. Accordingly, $\mathcal{C}_{3v} \supset \mathcal{C}_{sy}$ is a canonical subgroup chain, and the space $\mathcal{L}_{(0)}$ is irreducible. Therefore, out of x, y and z, we can construct the bases for the one– and two–dimensional irreps (3) and (0), respectively:

$$\psi_1^{(3)} = z\ , \quad \psi_1^{(0)} = x\ , \quad \psi_{-1}^{(0)} = y\ . \tag{3-78a}$$

Similarly, out of the six reducible basis vectors x^2, y^2, z^2, xy, xz and yz, we can obtain the following $\mathcal{C}_{3v} \supset \mathcal{C}_{sy}$ irreducible bases;

$$\begin{aligned} &\psi_1^{(3)1} = x^2 + y^2\ , && \psi_1^{(3)2} = z^2, \\ &\psi_1^{(0)1} = \rho^2 \cos 2\varphi = x^2 - y^2\ , && \psi_1^{(0)2} = xz\ , \\ &\psi_{-1}^{(0)1} = \rho^2 \sin 2\varphi = -2xy\ , && \psi_{-1}^{(0)2} = yz\ . \end{aligned} \tag{3-78b}$$

This shows that the irreps (3) and (0) both occur twice.

Ex. 3.3. Show that the $\mathcal{C}_{3v} \supset \mathcal{C}_{sy}$ irreducible bases are:

$$\begin{aligned} &\psi^{(3)} = \rho^m \cos m\varphi, && \psi^{(-3)} = \rho^m \sin m\varphi, \quad m = 0, 3, 6, \ldots, \\ &\psi_1^{(0)} = \rho^m \cos m\varphi, && \psi_{-1}^{(0)} = \rho^m \sin m\varphi, \quad m = 1, 2, 4, 5, \ldots. \end{aligned}$$

Ex. 3.4. Construct the $\mathcal{C}_{3v} \supset \mathcal{C}_3$ irreducible basis which is linear in x and y, and find the corresponding irreducible matrices.

Ex. 3.5. Construct the irreducible basis of $\mathcal{C}_{4v}$ from the polynomials of degree one and two in x, y and z, and find the irreducible matrices for the following two subgroup chains (using Fig. 1.1-3 and the result of Ex. 3.2):

$$(a)\quad \mathcal{C}_{4v} \supset (e, \sigma_4)\ , \qquad (b)\quad \mathcal{C}_{4v} \supset \mathcal{C}_4\ .$$

3.4.2. The group S_2

Suppose that there are two electrons, one with spin up (α) and the other with spin down (β). There are two possible states in the spin space,

$$\psi_1 = |\alpha\beta\rangle = \chi_\alpha(1)\chi_\beta(2)\ , \quad \varphi_2 = |\beta\alpha\rangle = \chi_\beta(1)\chi_\alpha(2)$$

which form a reducible (the regular) rep of S_2. The CSCO of S_2 is $C = (12)$. The eigenfunctions of C are easily found; they are

$$\psi^{(1)} = \sqrt{\tfrac{1}{2}}(\varphi_1 + \varphi_2)\ , \quad \psi^{(-1)} = \sqrt{\tfrac{1}{2}}(\varphi_1 - \varphi_2)\ . \tag{3-79a}$$

Those are the basis vectors for the two one-dimensional irreps (1) and (−1). $\psi^{(1)}(\psi^{(-1)})$ is symmetric (anti-symmetric) under the interchange of the spin coordinate indices 1 and 2, and is labelled conventionally by the so-called *Young tableau* $\boxed{1\,2}$ $\left(\begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline \end{array}\right)$ [to be discussed extensively in Sec. 4.3]. Thus equation (3.79a) can be written as

$$|\boxed{1\,2}\rangle = \sqrt{\tfrac{1}{2}}(\varphi_1 + \varphi_2)\ , \qquad \left|\begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline \end{array}\right\rangle = \sqrt{\tfrac{1}{2}}(\varphi_1 - \varphi_2)\ . \tag{3-79b}$$

3.4.3. The group S_3 in the configuration $\alpha^2\beta$

We now have three electrons in the configuration $\alpha^2\beta$. The three possible states

$$\varphi_1 = |\alpha\alpha\beta\rangle\ , \quad \varphi_2 = |\alpha\beta\alpha\rangle\ , \quad \varphi_3 = |\beta\alpha\alpha\rangle\ , \tag{3-80a}$$

carry a 3-dimensional rep of S_3. There are two ways of reducing this rep: (1) using the EFM, (2) using the projection operator method.

(1) The EFM. The CSCO of S_3 is

$$C = C(3) = (12) + (23) + (13)\ . \tag{3-80b}$$

The effect of the permutations (ij) on φ_l is given in Table 3.4.

Table 3.4. The effect of the permutations (ij) on φ_l.

$(ij)\varphi_l$ \ φ_l	$\varphi_1=\|\alpha\alpha\beta\rangle$	$\varphi_2=\|\alpha\beta\alpha\rangle$	$\varphi_3=\|\beta\alpha\alpha\rangle$
(12)	φ_1	φ_3	φ_2
(23)	φ_2	φ_1	φ_3
(13)	φ_3	φ_2	φ_1

Let $\varphi^{(\nu)} = a_1\varphi_1 + a_2\varphi_2 + a_3\varphi_3$. From Eqs. (3-75a), (3-80) and Table 3.4, we have

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \nu \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}\ . \tag{3-81}$$

This result gives a unique eigenvector for the single root $\nu = 3$, namely,

$$\psi^{(3)} = \left|\boxed{1}\boxed{2}\boxed{3}\right\rangle = \sqrt{\tfrac{1}{3}}(\varphi_1 + \varphi_2 + \varphi_3) \ . \tag{3-82}$$

This describes the totally symmetric or identity rep of S_3, $D^{(3)}(R_a) = 1$. The irreducible basis is traditionally labelled by the Young tableau $\boxed{1}\boxed{2}\boxed{3}$.

From (3-81) we also have a double root $\nu = 0$. We know from Sec. 3.4.1 that $\nu = 0$ is a two-dimensional irrep of $\mathcal{C}_{3v}$. Since S_3 is isomorphic to $\mathcal{C}_{3v}$, the double root $\nu = 0$ of (3-81) must correspond to a two-dimensional irrep of S_3 also. Substituting $\nu = 0$ into (3-81), we only get one independent equation

$$a_1 + a_2 + a_3 = 0 \ . \tag{3-83}$$

Clearly the solutions to (3-83) are not unique. Any two independent solutions yields a two-dimensional irrep of S_3. For example, we may have the following three sets of solutions giving rise to three reps $D^{(0)}, D^{(0)'}$ and $D^{(0)''}$,

$$\begin{cases} \psi_1^{(0)} = \sqrt{\frac{1}{6}}(2\varphi_1 - \varphi_2 - \varphi_3) \ , \\ \psi_{-1}^{(0)} = \sqrt{\frac{1}{2}}(\varphi_2 - \varphi_3) \ . \end{cases} \quad \begin{cases} \psi_1^{'(0)} = \sqrt{\frac{1}{6}}(\varphi_1 + \varphi_2 - 2\varphi_3) \ , \\ \psi_{-1}^{'(0)} = \sqrt{\frac{1}{2}}(\varphi_1 - \varphi_2) \ . \end{cases}$$

$$\begin{cases} \psi_1^{''(0)} = \sqrt{\frac{1}{6}}(\varphi_1 - 2\varphi_2 + \varphi_3) \ , \\ \psi_{-1}^{''(0)} = \sqrt{\frac{1}{2}}(\varphi_1 - \varphi_3) \ . \end{cases} \tag{3-84}$$

The three sets of basis here are related to one another by similarity transformations, so the irreps $D^{(0)}, D^{(0)'}$ and $D^{(0)''}$ are equivalent. This shows that the CSCO of G only determine the irreps up to an equivalence.

To fix the irreducible basis $\psi_m^{(\nu)}$ completely, we usually require that it also belongs to a definite irrep of the subgroup S_2, that is we need the $S_3 \supset S_2$ basis. According to Theorem 3.17 , it is necessarily a simultaneous eigenfunction of $C(3)$ and $C(2), C_2 = (12)$ being the CSCO of S_2:

$$\begin{pmatrix} C(3) \\ C(2) \end{pmatrix} \psi_m^{(\nu)} = \begin{pmatrix} \nu \\ m \end{pmatrix} \psi_m^{(\nu)} \ . \tag{3-85}$$

Using Table 3.4, the solutions to the eigenequation of $C(2)$ are

$$m = 1, \quad \text{double root} \ , \quad a_2 = a_3 \ , \tag{3-86}$$

$$m = -1, \quad \text{single root} \ , \quad a_1 = 0, \quad a_2 = -a_3 \ . \tag{3-87}$$

Combining these with Eq. (3-83), we obtain two simultaneous eigenfunctions which are precisely $\psi_1^{(0)}$ and $\psi_{-1}^{(0)}$ of Eq. (3-84). The totally symmetric basis $\psi^{(3)}$ is an eigenvector of $C(2)$ with eigenvalue $+1$ and can therefore be rewritten as $\psi_1^{(3)}$.

Summarizing, the CSCO of $S_3, C(3)$, is a CSCO in the class space of S_3, but it is no longer a CSCO in the configuration space $\{\varphi_i\}$. $(C(3), C(2))$ is the CSCO for the canonical subgroup chain $S_3 \supset S_2$, which is called the CSCO–II of S_3 (for a general definition, see Sec. 3.8), and is a CSCO in any multiplicity–free rep space of S_3.

In solving eigenequations (3-85), we adopted the procedure of first solving the part associated with $C(3)$, and then the part associated with $C(2)$. In practice, for hand calculations, it is more convenient to do the opposite. For example, from Eq. (3-86) we obtain the solution $a_2 = a_3$ for $m = 1$. Let us choose a_1 and a_2 as the independent variables. From (3-81) pick out two equations involving a_2 and a_3, and use $a_2 = a_3$ to eliminate the variable a_3. As a result, we obtain the following two equations

$$\begin{cases} a_1 + 2a_2 = \nu a_1 \ , \\ a_1 + 2a_2 = \nu a_2 \ , \end{cases} \quad \begin{vmatrix} 1-\nu & 2 \\ 1 & 2-\nu \end{vmatrix} = \nu(\nu - 3) = 0 \ . \tag{3-88}$$

The solutions are immediately found to be

$$\begin{aligned}(\nu,m)&=(3,1)\ ,\quad a_1=a_2=a_3\ ,\\ (\nu,m)&=(0,1)\ ,\quad a_1=-2a_2=-2a_3\ .\end{aligned}\tag{3-89}$$

Traditionally, the two basis vectors of the two-dimensional irrep of S_3 are labelled by the following two Young tableaux,

$$\begin{aligned}\psi_1^{(0)}&=\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}\right\rangle=\sqrt{\frac{1}{6}}(2\varphi_1-\varphi_2-\varphi_3)\ ,\\ \psi_{-1}^{(0)}&=\left|\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}\right\rangle=\sqrt{\frac{1}{2}}(\varphi_2-\varphi_3)\ .\end{aligned}\tag{3-90}$$

$\psi_1^{(0)}(\psi_{-1}^{(0)})$ is symmetric (anti-symmetric) in the indices 1 and 2. Note that from (3-82) and (3-90) we can get the transformation matrix from the reducible basis $\{\varphi_i\}$ to the irreducible bases $(\psi_1^{(3)},\psi_1^{(0)},\psi_{-1}^{(0)})$ and the matrix is precisely the one given by Eq. (2-99).

With the help of (2-47b) and Table 3.4, we can get the rep matrices for the irrep (0) of S_3 in the basis $(\psi_1^{(0)},\psi_{-1}^{(0)})$,

$$D^{(0)}(e)=\begin{pmatrix}1&0\\0&1\end{pmatrix},\ D^{(0)}(12)=\begin{pmatrix}1&0\\0&-1\end{pmatrix},\ D^{(0)}(23)=\frac{1}{2}\begin{pmatrix}-1&\sqrt{3}\\\sqrt{3}&1\end{pmatrix}.\tag{3-91a}$$

Using (1-8b) and (1-9), we can write the remaining matrices

$$D^{(0)}(13)=\frac{1}{2}\begin{pmatrix}-1&-\sqrt{3}\\-\sqrt{3}&1\end{pmatrix},\quad D^{(0)}(123)=\tilde{D}^{(0)}(132)=\frac{1}{2}\begin{pmatrix}-1&\sqrt{3}\\-\sqrt{3}&-1\end{pmatrix}\ .\tag{3-91b}$$

Notice that the irreducible basis in (3-90) does not have a definite symmetry with respect to the interchange of the coordinate indices 1 and 3, or 2 and 3. This is because

$$[(12),\,(23)]\neq 0\ ,\quad [(12)\ ,\,(13)]\neq 0\ ,\tag{3-92}$$

and thus the three transpositions (12), (23) and (13) cannot be diagonalized simultaneously.

It can be shown that $(\psi_1^{'(0)},\psi_{-1}^{'(0)})$ and $(\psi_1^{''(0)},\psi_{-1}^{''(0)})$ in Eq. (3-84) are the irreducible bases of $S_3\supset S_2(23)$ and $S_3\supset S_2(13)$, respectively.

(2) The projection operator method. Applying the operator $Q^{(3)}$ of (3-44a) to φ_1, we have

$$\psi^{(3)}=aQ^{(3)}\varphi_1=\sqrt{\tfrac{1}{3}}(\varphi_1+\varphi_2+\varphi_3),\tag{3-93}$$

where a is a constant. Applying $Q^{(3)}$ to φ_2 and φ_3 gives the same result. Therefore, $Q^{(3)}$ projects out a one-dimensional rep space. Applying $Q^{(0)}$ to φ_1,φ_2 and φ_3 we get three functions

$$\begin{aligned}\psi_1^{(0)}&=bQ^{(0)}\varphi_1=\sqrt{\tfrac{1}{6}}(2\varphi_1-\varphi_2-\varphi_3)\ ,\\ \psi_2^{(0)}&=bQ^{(0)}\varphi_2=\sqrt{\tfrac{1}{6}}(2\varphi_2-\varphi_1-\varphi_3)\ ,\\ \psi_3^{(0)}&=bQ^{(0)}\varphi_3=\sqrt{\tfrac{1}{6}}(2\varphi_3-\varphi_1-\varphi_2)\ ,\end{aligned}\tag{3-94}$$

where only two of them are linearly independent. Hence $Q^{(0)}$ projects out a two-dimensional rep space. Equation (3-93) is identical to (3-82), however (3-94) differs from (3-90) in that (a) Eq. (3-90) is the $S_3\supset S_2$ basis while (3-94) is not; (b) the basis vectors in (3-90) are orthogonal, while those of Eq. (3-94) are not.

The advantage of the EFM is that once the CSCO of G and $G(s)$ are known, we can solve the eigenequation (3-77b) directly to obtain the $G \supset G(s)$ irreducible basis without first finding $Q^{(\nu)}$.

More will be said about the projection operator method in Sec. 3.13.

Ex. 3.6. Show that in the state $\psi_1^{(0)} = \left|\begin{array}{|c|c|}\hline 1&2\\\hline\end{array}\atop\begin{array}{|c|}\hline 3\\\hline\end{array}\right\rangle$ the probabilities of the particles 1 and 3 being symmetric and of the particles 2 and 3 being symmetric, are each equal to $\frac{1}{4}$, while in the state $\psi_{-1}^{(0)} = \left|\begin{array}{|c|c|}\hline 1&3\\\hline\end{array}\atop\begin{array}{|c|}\hline 2\\\hline\end{array}\right\rangle$, the same probabilities are each equal to $\frac{3}{4}$.

Ex. 3.7. Use the EFM to reduce the three-dimensional rep carried by $\{|\alpha\beta\beta\rangle, |\beta\alpha\beta\rangle, |\beta\beta\alpha\rangle\}$.

3.4.4. The group S_3 in the configuration $\alpha\beta\gamma$

Suppose that we have three particles in the configuration $\alpha\beta\gamma$. The system has six possible states $\varphi_1, \ldots, \varphi_6$ (see Eq. (2-70)), which carry the regular rep of S_3. The irreducible basis $\psi_m^{(\nu)} = \sum_i u_i \varphi_i$ satisfies the eigenequations (3-85). To find the coefficients u_i, we have to diagonalize the regular representation matrices $D(C(3)) = D(12) + D(23) + D(13)$, and $D(C(2)) = D(12)$, simultaneously. Using (2-71), we find the eigenequations of $C(3)$ and $C(2)$ to be

$$\begin{pmatrix} -\nu & 1 & 1 & 1 & 0 & 0 \\ 1 & -\nu & 0 & 0 & 1 & 1 \\ 1 & 0 & -\nu & 0 & 1 & 1 \\ 1 & 0 & 0 & -\nu & 1 & 1 \\ 0 & 1 & 1 & 1 & -\nu & 0 \\ 0 & 1 & 1 & 1 & 0 & -\nu \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{pmatrix} = 0, \quad \begin{pmatrix} -m & 1 & 0 & 0 & 0 & 0 \\ 1 & -m & 0 & 0 & 0 & 0 \\ 0 & 0 & -m & 0 & 0 & 1 \\ 0 & 0 & 0 & -m & 1 & 0 \\ 0 & 0 & 0 & 1 & -m & 0 \\ 0 & 0 & 1 & 0 & 0 & -m \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{pmatrix} = 0. \quad \text{(3-95a,b)}$$

The eigenvalues ν can be obtained by inspection. For $\nu = 0$, the rank of the matrix in (3-95a) is two; therefore $\nu = 0$ is a four-fold root. According to Theorem 3.11, in the group space $C(3)$ has the same eigenvalues 3, 0, and -3 as those of the class space. Thus the matrix in (3-95a) has another two single roots $\nu = \pm 3$ with the eigenvectors

$$\psi^{(3)} = \psi_1^{(3)} = \left|\begin{array}{|c|c|c|}\hline 1&2&3\\\hline\end{array}\right\rangle = \sqrt{\tfrac{1}{6}}(\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4 + \varphi_5 + \varphi_6) ,$$

$$\psi^{(-3)} = \psi_{-1}^{(-3)} = \left|\begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\hline\end{array}\right\rangle = \sqrt{\tfrac{1}{6}}(\varphi_1 - \varphi_2 - \varphi_3 - \varphi_4 + \varphi_5 + \varphi_6) . \qquad \text{(3-96)}$$

It is easy to verify that $\psi^{(3)}(\psi^{(-3)})$ is totally symmetric (anti-symmetric) and therefore belongs to the irrep $m = 1$ (-1) of S_2. The totally anti-symmetric rep and is called the *alternating representation* of S_3. In the anti-symmetric rep all odd (even) permutations are represented by $-1(+1)$,

$$D(12) = D(23) = D(13) = -1, \quad D(e) = D(123) = D(132) = 1 . \qquad \text{(3-98)}$$

The alternating rep of S_3 is labelled by the Young tableau $\begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\hline\end{array}$.

For the four-fold root $\nu = 0$, from (3-95a) we only get two independent equations, namely,

$$\nu = 0: \quad u_1 + u_5 + u_6 = 0 , \quad u_2 + u_3 + u_4 = 0 . \qquad \text{(3-99)}$$

Furthermore, from (3-95b) we have three equations:

$$m = \pm 1: \; u_1 = \pm u_2, \; u_3 = \pm u_6, \; u_4 = \pm u_5 . \qquad \text{(3-100)}$$

Combining the last two equations, for $(\nu, m) = (0, 1)$ and for $(\nu, m) = (0, -1)$ we obtain only one independent equation

$$(\nu, m) = (0, 1): \quad u_1 + u_3 + u_4 = 0 \,, \tag{3-101}$$

$$(\nu, m) = (0, -1): \quad u_1 - u_3 - u_4 = 0 \,. \tag{3-102}$$

Therefore, the solutions are not unique. Why is this so? From Eq. (3-91) we know that $\nu = 0$ is a two-dimensional irrep, $h_\nu = 2$. Here $\nu = 0$ is a four-fold root, that is $M_\nu = 4$. Since $M_\nu = \tau_\nu h_\nu$, the irrep (0) must occur twice ($\tau_\nu = 2$) in the regular rep of S_3. In other words, in the decomposition of the group space of S_3

$$L_g \equiv L_{(3)} + L_{(0)} + L_{(-3)} \,, \tag{3-103}$$

the four-dimensional eigenspace of $C(3)$ can be reduced into a direct sum of two equivalent irreducible spaces of dimension 2:

$$L_{(0)} = L_{(0)1} \oplus L_{(0)2} \,. \tag{3-104}$$

How does one decompose the eigenspace $L_{(0)}$, or more generally, how does one decompose the eigenspace $L_{(\nu)}$ of the CSCO of G? According to Theorem 2.7, if we can find a new operator $\overline{C}_1$ which commutes with G, then the eigenspace $L_{(\nu)}$ can be further decomposed into a direct sum of the eigenspaces of $\overline{C}_1$,

$$L_{(\nu)} = \sum_{k_1} \oplus L_{(\nu)k_1}, \quad \overline{C}_1 L_{(\nu)k_1} = k_1 L_{(\nu)k_1} \,. \tag{3-105}$$

If the subspace $L_{(\nu)k_1}$ is still reducible, then we need to find another operator $\overline{C}_2$ which commutes with both G, and $\overline{C}_1$, and decompose $L_{(\nu)k_1}$ into a direct sum of the eigenspaces of $\overline{C}_2$, and so on until we find a set of operators $\overline{C}(s) = (\overline{C}_1 \overline{C}_2 \ldots)$ such that the simultaneous eigenspaces of $\overline{C}(s)$ are irreducible. The eigenvalue $k = (k_1, k_2, \ldots)$ of $\overline{C}(s)$ thus provides new label to distinguish the equivalent irreps contained in $L_{(\nu)}$.

By Theorems 3.1 and 3.4, we cannot find such operators from the group G. In other words, it is impossible to use the remaining class operators of G which are not contained in the CSCO of G to further decompose the eigenspace $L_{(\nu)}$. Therefore, we have to search for another group $\overline{G}$ which commutes with G and thus will provide some new operators with which to decompose the eigenspace $L_{(\nu)}$. We will begin, in the following section, by first solving this problem for the permutation group.

3.5. The State Permutation Group

Suppose that there are n particles occupying n distinct single particle states, $i_1, i_2, \ldots, i_n$. The state

$$\begin{aligned} \Psi(X) \equiv \Psi(x_1, \ldots, x_n) &= \varphi_{i_1}(x_1)\varphi_{i_2}(x_2) \ldots \varphi_{i_n}(x_n) \\ &= |\omega_0\rangle = \prod_{a=1}^{n} \varphi_{i_a}(x_a) = |i_1 i_2 \ldots i_n\rangle \end{aligned} \tag{3-106}$$

is referred to as the *normal order state* , in which the kth particle is in the kth single particle state. The ordering of the single particle states is specified from the beginning. For example, for the orbital angular momentum $l = 1$, one may specify $m = 1, 0, -1$ as the states i_1, i_2, i_3, respectively. However, once the ordering is specified, we must abide by it through the whole analysis. Under the above specification, $|10-1\rangle$ is a normal order state, and all the other states, such as $|01-1\rangle, |-101\rangle$ are not.

Up to now, the element p of a permutation group S_n is defined as a permutation of the subscripts of the coordinates $\{x_a\}$. We now introduce another kind of permutation, designated

by the script letter $\wp$, which permutes the subscripts of the single particle states $\{i_a\}$, and is called a state permutation (Bohr 1969). All the permutations of the n state indices form a group, called the *state permutation group* $\mathcal{S}_n$. For example

$$\wp_{123}|i_1 i_2 i_3\rangle = |i_2 i_3 i_1\rangle \ , \quad \wp_{23}|i_2 i_3 i_1\rangle = |i_3 i_2 i_1\rangle \ , \tag{3-107a}$$

in contrast to the coordinate permutations

$$p_{123}|i_1 i_2 i_3\rangle = |i_3 i_1 i_2\rangle \ , \quad p_{23}|i_2 i_3 i_1\rangle = |i_2 i_1 i_3\rangle \ . \tag{3-108}$$

For simplicity in notation, we often use $\alpha, \beta, \gamma, \delta, \ldots$ in place of the $\{i_a\}$. Thus $\wp_{12} = (\alpha\beta)$ denotes an interchange of α and β, while $\wp_{123} = (\alpha\beta\gamma)$ denotes a cycle permutation $\alpha \to \beta \to \gamma \to \alpha$. With this notation, Eq. (3-107a) becomes

$$\wp_{123}|\alpha\beta\gamma\rangle = |\beta\gamma\alpha\rangle \ , \quad \wp_{23}|\beta\gamma\alpha\rangle = |\gamma\beta\alpha\rangle \ . \tag{3-107b}$$

The permutation group $\mathcal{S}_n$ has the following properties.

1. $\mathcal{S}_n$ and S_n are isomorphic.
2. $\mathcal{S}_n$ and S_n commute, that is

$$[p_a, \wp_b] = 0 \ . \tag{3-109}$$

3. For the normal order state we have

$$p|\omega_0\rangle = \wp^{-1}|\omega_0\rangle \ . \tag{3-110}$$

The first and second points are self evident, and the third point is proved as follows. Let $p = \binom{a}{a'}$, so that p is the coordinate transformation $x_a \to x_{a'}$ and let $\wp = \binom{i_a}{i_{a'}}$, so that $\wp$ performs the change $i_a \to i_{a'}$. We then have

$$p\wp|\omega_0\rangle = p\wp \prod_{a=1}^{n} \varphi_{i_a}(x_a) = \prod_{a'=1}^{n} \varphi_{i_{a'}}(x_{a'}) = |\omega_0\rangle \ . \tag{3-111}$$

This proves Eq. (3-110).

Remark 1: Equation (3-110) does not imply that $p = \wp^{-1}$. It only shows that when acting on the normal order state, $p = \wp^{-1}$, while for other states, $p \neq \wp^{-1}$ in general.

Remark 2: The term state permutation was also used in Weyl (1946) and Hamermesh (1962). Although their definitions of the state permutation appear the same as that given here, that is as a permutation of the state indices, the two definitions are actually different. In our case each single particle state is assigned a definite index from the beginning, regardless of which particle occupies it. In Weyl (1946) and Hamermesh (1962), the state index k is assigned to the single particle state occupied by the k–th particle regardless of which single particle state it is in. For example, in the product state $|10-1\rangle$, they took $i_1 = 1, i_2 = 0, i_3 = -1$, while in the product state $|-101\rangle$, they took $i_1 = -1, i_2 = 0, i_3 = 1$. According to their definition, any n–particle product state is always of the form $\prod_{a=1}^{n} \varphi_{i_a}(x_a)$. Therefore what they called a state permutation $\mathbf{p}$ is always equal to the inverse of the coordinate permutation p, that is

$$\mathbf{p} = p^{-1} \ . \tag{3-112}$$

So the group $\{\mathbf{p}\}$ is nothing new, it is essentially the coordinate permutation group, and is useless for our current purposes. We always use Eq. (3-107) as the definition for state permutations.

Applying the $n!$ elements of S_n or $\mathcal{S}_n$ to the normal order state $\Psi_0 = |\omega_o\rangle$, we obtain the $n!$ states

$$\varphi_a = p_a|\omega_0\rangle = \wp_a^{-1}|\omega_0\rangle = p_a|i_1, i_2, \ldots, i_n\rangle \ . \tag{3-113}$$

They form a basis for the regular rep of S_n as well as of $\mathcal{S}_n$.

Using (3-109) and the ambivalence of all classes of the permutation group, we have

$$\mathcal{C}_j\varphi_a = \mathcal{C}_j p_a|\omega_0\rangle = p_a\mathcal{C}_j|\omega_0\rangle = p_a C_{j'}|\omega_0\rangle = p_a C_j|\omega_0\rangle = C_j p_a|\omega_0\rangle = C_j\varphi_a \ , \tag{3-114}$$

where $C_{j'}$ is defined by Eq. (3-38). Since φ_a in the above is an arbitrary function,

$$\mathcal{C}_j = C_j \ , \quad j = 1,2,\ldots,N \ . \tag{3-115a}$$

Therefore the CSCO of $\mathcal{S}_n$ and S_n are equal, that is

$$\mathcal{C}(n) = C(n) \ . \tag{3-115b}$$

According to Theorem 3.16 , this implies that if $\psi^{(\nu)}$ belongs to the irrep (ν) of S_n, it must also belong to the irrep (ν) of $\mathcal{S}_n$.

From the last two results, the class operators of $\mathcal{S}_n$ do not give any new operators. Fortunately, the class operators $\mathcal{C}_k(i)$ of the subgroup $\mathcal{S}_i$ are not equal to the class operators $C_k(i)$ of $S_i, i = n-1,\ldots,2$. This can be seen from the fact that $[\mathcal{C}_k(i), S_n] = 0$, while $[C_k(i), S_n] \neq 0$. We use $\mathcal{C}(i)$ to denote the CSCO of the subgroup $\mathcal{S}_i$ of the state permutation group $\mathcal{S}_n$. Then the set of operators $\mathcal{C}(s) = (\mathcal{C}(n-1), \mathcal{C}(n-2), \ldots, \mathcal{C}(2))$ provides a set of new operators, which can be used to decompose the eigenspace of the CSCO of S_n. Before discussing the general case, we return to the unfinished problem of Sec. 3.4 on the reduction of the rep space $L_{(0)}$ of S_3.

3.6. Reduction of the Regular Rep of S_3

First Approach. With the new operator $\mathcal{C}(2) = \wp_{12}$, the eigenequation (3-85) is extended to

$$\begin{pmatrix} C(3) \\ C(2) \\ \mathcal{C}(2) \end{pmatrix} \psi_m^{(\nu)k} = \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} \psi_m^{(\nu)k} \ , \quad \psi_m^{(\nu)k} = \sum_{i=1}^{6} u_i\varphi_i \ , \tag{3-116}$$

where the φ_i were defined in (2-70). From the definition $\wp_{12} = (\alpha\beta)$, we have

$$\wp_{12}|\alpha\beta\gamma\rangle = |\beta\alpha\gamma\rangle \ , \ \wp_{12}|\gamma\beta\alpha\rangle = |\gamma\alpha\beta\rangle \ , \ \wp_{12}|\alpha\gamma\beta\rangle = |\beta\gamma\alpha\rangle \ ,$$

or

$$\wp_{12}\varphi_1 = \varphi_2 \ , \ \wp_{12}\varphi_3 = \varphi_5 \ , \ \wp_{12}\varphi_4 = \varphi_6 \ . \tag{3-117}$$

Since $\wp_{12}$ squares to $+1$, it has eigenvalues $k = \pm 1$. From (3-116) and (3-117) we obtain

$$k = \pm 1 : \ u_1 = \pm u_2, \ u_3 = \pm u_5, \ u_4 = \pm u_6 \ . \tag{3-118}$$

Combining Eqs. (3-110), (3-101), (3-102) and (3-118), we obtain the following four eigenvectors $\psi_m^{(\nu)k}$

$$\begin{aligned}
\psi_1^{(0)1}(\alpha\beta\gamma) &= \left| \begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array} \ \begin{array}{|c|c|}\hline \alpha&\beta\\\hline \gamma\\\cline{1-1}\end{array} \right\rangle \\
&= \tfrac{1}{\sqrt{12}}[2(\varphi_1+\varphi_2) - (\varphi_3+\varphi_4+\varphi_5+\varphi_6)] \ . \\
\psi_{-1}^{(0)1}(\alpha\beta\gamma) &= \left| \begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array} \ \begin{array}{|c|c|}\hline \alpha&\beta\\\hline \gamma\\\cline{1-1}\end{array} \right\rangle = \tfrac{1}{2}[-\varphi_3+\varphi_4-\varphi_5-\varphi_6] \ , \\
\psi_1^{(0)-1}(\alpha\beta\gamma) &= \left| \begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array} \ \begin{array}{|c|c|}\hline \alpha&\gamma\\\hline \beta\\\cline{1-1}\end{array} \right\rangle = \tfrac{1}{2}[-\varphi_3+\varphi_4+\varphi_5+\varphi_6] \ , \\
\psi_{-1}^{(0)-1}(\alpha\beta\gamma) &= \left| \begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array} \ \begin{array}{|c|c|}\hline \alpha&\gamma\\\hline \beta\\\cline{1-1}\end{array} \right\rangle = \tfrac{1}{\sqrt{12}}[2(\varphi_1-\varphi_2)+\varphi_3+\varphi_4-\varphi_5-\varphi_6] \ .
\end{aligned} \tag{3-119a}$$

Since $C(3) = \mathcal{C}(3)$, Theorem 3.17 implies the eigenvectors $\psi_m^{(\nu)k}$ of (3-116) form an irreducible basis (ν, m) for the group chain $S_3 \supset S_2$, and an irreducible basis (ν, k), for the group chain $\mathcal{S}_3 \supset \mathcal{S}_2$.

In Sec. 3.4, we used tableaux filled with numbers, the Young tableaux, to designate a $S_3 \supset S_2$ irreducible basis. Analogously we use tableaux filled with single particle states α, β, γ, referred to as *Weyl tableaux* (see Sec. 4.8 for a general definition), to designate a $\mathcal{S}_3 \supset \mathcal{S}_2$ irreducible basis. Therefore, instead of the quantum numbers ν, m and k, we can use two tableaux, one Young tableau Y_m^ν and one Weyl tableau W_k^ν, to label a $S_3 \supset S_2$ and $\mathcal{S}_3 \supset \mathcal{S}_2$ irreducible basis. The totally symmetric (anti-symmetric) state in (3-96) [(3-97)] is also totally symmetric (anti-symmetric) in the state indices α, β and γ and can be labelled by two tableaux as

$$\psi_1^{(3)1}(\alpha\beta\gamma) = \left| \boxed{1}\boxed{2}\boxed{3} \quad \boxed{\alpha}\boxed{\beta}\boxed{\gamma} \right\rangle = \tfrac{1}{\sqrt{6}}[\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4 + \varphi_5 + \varphi_6]$$

$$\psi_{-1}^{(-3)-1}(\alpha\beta\gamma) = \left| \begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline 3 \\ \hline \end{array} \quad \begin{array}{|c|}\hline \alpha \\ \hline \beta \\ \hline \gamma \\ \hline \end{array} \right\rangle = \tfrac{1}{\sqrt{6}}[\varphi_1 - \varphi_2 - \varphi_3 - \varphi_4 + \varphi_5 + \varphi_6] \,, \tag{3-119b}$$

The pair of eigenvectors $(\psi_1^{(0)1}, \psi_{-1}^{(0)1})$ and $(\psi_1^{(0)-1}, \psi_{-1}^{(0)-1})$ form the two irreducible spaces $L_{(0)1}$ and $L_{(0)-1}$, respectively. It is easy to check that the irreducible matrices of S_3 in these two spaces are the same, and are identical to (3-91). Therefore, these two irreps, which are distinguished by the quantum number k of $\mathcal{C}(2)$, the CSCO of the state permutation group $\mathcal{S}_2$, are not only equivalent but also identical (due to our special choice for the phases of the solutions). The four-dimensional eigenspace $L_{(0)}$ of $C(3)$ is thus decomposed into a direct sum of the two eigenspaces of $\mathcal{C}(2)$,

$$L_{(0)} = L_{(0)1} \oplus L_{(0)-1} \,, \quad \mathcal{C}(2)L_{(0)k} = kL_{(0)k} \,. \tag{3-120}$$

The set of operators, $K = (C(3), C(2), \mathcal{C}(2))$, forms a CSCO in the regular rep space of S_3, and is called the CSCO-III of S_3 (for a general definition, see Sec. 3.8). The simultaneous eigenspaces of K are all one-dimensional. Thus the six-dimensional group space S_3 is fully decomposed into a direct sum of six one-dimensional spaces

$$L_g = \sum_{\nu m k} \oplus L_{(\nu)mk} \,. \tag{3-121}$$

Similarly, $(\psi_1^{(0)1}, \psi_1^{(0)-1})$ and $(\psi_{-1}^{(0)1}, \psi_{-1}^{(0)-1})$ form two irreducible spaces of $\mathcal{S}_3$. The irreducible matrices of $\mathcal{S}_3$ in these two spaces are also identical with (3-91). These two equivalent irreps of the state permutation group are distinguished by the quantum number of the operator $C(2)$, the CSCO of the coordinate permutation group S_2.

Second Approach. In the discussion above, we first solved the eigenequations of $C(3)$, and then those of $C(2)$ and $\mathcal{C}(2)$. For actual calculations, it is more convenient to first use the eigenequations of $C(2)$ and $\mathcal{C}(2)$ to eliminate the non-independent variables u_i and thus to reduce the order of the eigenequation of $C(3)$. We made a similar point in Sec 3.4.3. The concrete steps are as follows.

(a) Applying the operators $C(2) = (12)$ and $\mathcal{C}(2) = (\alpha\beta)$ to φ_i, we obtain Table 3.6-1, which in turn gives (3-122).

$$\begin{aligned} m = \pm 1 &: \; u_1 = \pm u_2 \,, \; u_3 = \pm u_6, \,, \; u_4 = \pm u_5 \,, \\ k = \pm 1 &: \; u_1 = \pm u_2 \,, \; u_3 = \pm u_5, \,, \; u_4 = \pm u_6 \,. \end{aligned} \tag{3-122}$$

Combining these two sets of equations, we get

$$(m,k) = (1,1) : \; u_1 = u_2 \,, \qquad u_3 = u_4 = u_5 = u_6 \,, \tag{3-123a}$$

$$(-1,-1) : \; u_1 = -u_2 \,, \qquad u_3 = u_4 = -u_5 = -u_6 \,, \tag{3-123b}$$

$$(1,-1) : \; u_1 = u_2 = 0 \,, \qquad u_3 = -u_4 = -u_5 = u_6 \,, \tag{3-123c}$$

$$(-1,1) : \; u_1 = u_2 = 0 \,, \qquad u_3 = -u_4 = u_5 = -u_6 \,. \tag{3-123d}$$

Table 3.6-1. The action of $C(2)$ and $\mathcal{C}(2)$ on the φ_i.

φ_i / $R\varphi_i$ / R	φ_1 $\lvert\alpha\beta\gamma\rangle$	φ_2 $\lvert\beta\alpha\gamma\rangle$	φ_3 $\lvert\gamma\beta\alpha\rangle$	φ_4 $\lvert\alpha\gamma\beta\rangle$	φ_5 $\lvert\gamma\alpha\beta\rangle$	φ_6 $\lvert\beta\gamma\alpha\rangle$
(12)	φ_2	φ_1	φ_6	φ_5	φ_4	φ_3
$\wp 12$	φ_2	φ_1	φ_5	φ_6	φ_3	φ_4

(b) For $(m,k) = (1,1)$ and $(-1,-1)$ only two independent variables are left, which may be chosen to be u_1 and u_3. Two more equations involving u_1 and u_3 are needed. They can be found from the eigenequation of $C(3)$. To this end, according to (3-75b), we only need to know the effect of $C(3)$ on the states φ_1 and φ_3, which are listed in Table 3.6-2.

Table 3.6-2. The action of $C(3)$ on φ_1 and φ_3.

p / $p\varphi_i$ / φ_i	(12)	(13)	(23)
φ_1	φ_2	φ_3	φ_4
φ_3	φ_6	φ_1	φ_5

Using Eq. (3-75b) and Table 3.6-2, we obtain

$$u_2 + u_3 + u_4 = \nu u_1 \ , \quad u_1 + u_5 + u_6 = \nu u_3 \ . \tag{3-124}$$

Combining (3-123a) and (3-124) leads to

$$\begin{aligned} u_1 + 2u_3 &= \nu u_1 \ , \\ u_1 + 2u_3 &= \nu u_3 \ , \end{aligned} \quad \begin{vmatrix} 1-\nu & 2 \\ 1 & 2-\nu \end{vmatrix} = \nu(\nu-3) = 0 \ . \tag{3-125}$$

From (3-125) and (3-123a), we obtain the eigenvectors $\psi_1^{(3)1}$ and $\psi_1^{(0)1}$, which have already been given in (3-119).

Combining (3-124) and (3-123b) leads to

$$\begin{aligned} -u_1 + 2u_3 &= \nu u_1 \ , \\ u_1 - 2u_3 &= \nu u_3 \ , \end{aligned} \quad \begin{vmatrix} -1-\nu & 2 \\ 1 & -2-\nu \end{vmatrix} = \nu(\nu+3) = 0 \ . \tag{3-126}$$

From (3-126) and (3-123b), we obtain the eigenvectors $\psi_{-1}^{(-3)-1}$ and $\psi_{-1}^{(0)-1}$, which were also given in Eq. (3-119).

For $(m,k) = (1,-1)$ and $(-1,1)$, Eqs. (3-123c) and (3-123d) alone give two unique eigenvectors, which can be identified as $\psi_1^{(0)-1}$ and $\psi_{-1}^{(0)1}$. They are identical to the expressions given in (3-119a).

3.7. The Intrinsic Group

In Secs. 3.4-3.6, we have discussed the reduction of the rep of S_3 carried by the product states. We now proceed to generalize this procedure to a general theory. For the coordinate permutation group S_n, we have used a state permutation group $\mathcal{S}_n$ that is isomorphic to and commuting with S_n. The method is generalized to any group G by finding a group $\overline{G}$ that is anti-isomorphic (since there is no essential difference between isomorphism and anti-isomorphism) to G and commutes with it.

3.7.1. Definition of the intrinsic group

Definition 3.3: For each element R of a group G, we can define a corresponding operator $\overline{R}$ in the group space L_g through the following *defining equation*:

$$\overline{R}S = SR\,, \quad \text{for all } S \in L_g\,. \tag{3-127}$$

The group formed by the collection of the operators $\overline{R}$ is called the *intrinsic group* of G, or simply the intrinsic group $\overline{G}$ if no confusion will arise.

Equation (3-127) states that the operation of $\overline{R}$ on a vector S in L_g changes it into another vector SR. As such, (3-127) is a *defining* equation for the operator $\overline{R}$ rather than an operator identity. That is to say, it is not permissible to multiply (3-127) from the right by another vector T of L_g,

$$\overline{R}ST \neq SRT\,. \tag{3-128}$$

Instead, we should regard ST as a new vector in L_g and then use (3-127) to obtain

$$\overline{R}ST = \overline{R}(ST) = (ST)R\,, \tag{3-129a}$$

or more generally,

$$\overline{R}(R_aR_b\cdots R_c) = (R_aR_b\cdots R_c)R\,. \tag{3-129b}$$

From the above one can say that the intrinsic operator $\bar{R}$ is the operator R acting from the right, and it is in fact the inverse $\mathcal{R}_R^{-1}$ of the standard right action operator $\mathcal{R}_R$ of Coleman 1968.

From (3-127) and (3-129) one has

$$S\overline{R}T = STR = \overline{R}ST\,, \quad \text{for all } T \in L_g\,. \tag{3-130}$$

Since T is an arbitrary vector in L_g, from (3-129a) and (3-130) one has the operator identity

$$\overline{R}S = S\overline{R}\,, \tag{3-131a}$$

or

$$[\overline{R}, S] = 0\,. \tag{3-131b}$$

Therefore the operators in $\overline{G}$ commute with those in G.

Notice the difference between (3-127) and (3-131a). The latter is an identity relation, while the former is not. In (3-127) S is regarded as a vector in L_g, whereas in (3-131a) S is an operator in L_g. The rule for determining whether a group element S is to be regarded as a basis vector or as an operator is very simple. If S is the last element after an intrinsic group operator, then S should be looked upon as a basis vector; if S is followed by another group element of G, then S should be regarded as an operator.

We now show that the operators $\overline{R}$ do form a group. Suppose that the multiplication relation for the group G is

$$RS = U\,. \tag{3-132a}$$

From Eqs. (3-127) and (3-129) we have

$$\overline{S}\,\overline{R}T = \overline{S}(TR) = (TR)S = TU = \overline{U}T\,. \tag{3-133}$$

Since T is any vector in L_g, one has

$$\overline{S}\,\overline{R} = \overline{U}\,. \tag{3-132b}$$

Therefore, there is a one–to–one correspondence between the elements $\overline{R}$ and R, and (3-132) shows that the collection of $\overline{R}$ forms a group $\overline{G}$ which is anti–isomorphic to and commutes with the group G.

3.7.2. The intrinsic state (regular rep case)

The action of the intrinsic group elements in configuration space is easily worked out in the case of a regular representation based on a function Ψ_0 in configuration space without any symmetry. As assumed in Sec. 2.6.1, under the action of the g elements of G, it gives g orthonormal functions

$$\varphi_a = R_a\Psi_0 \ , \quad a = 1, 2, \ldots g \ , \tag{3-134}$$

which carry the regular rep of G. As mentioned before, $\overline{R}S = SR$ is not an identity. Therefore, it does not hold when acting on all of these g functions. However, we may require it to hold when acting on one of them, say $\Psi_0(X)$,

$$\overline{R}S\Psi_0(X) = SR\Psi_0(X) \ . \tag{3-135}$$

Letting S be the identity element we have

$$\overline{R}\Psi_0(X) = R\Psi_0(X) = \Psi_0(R^{-1}X) \ . \tag{3-136}$$

In this way, we have defined the action of $\overline{R}$ on the chosen state $\Psi_0(X)$. We call the state $\Psi_0(X)$ which satisfies (3-136) the *intrinsic state* of the group G . Equation (3-136) shows that when acting on the intrinsic state, $\overline{R}$ is equivalent to R. The physical interpretation of the intrinsic state for the rotation group will be given in Sec. 6.6.

We now show that once an intrinsic state is chosen, the remaining $g-1$ states of the configuration states are no longer intrinsic. From (3-127) and (3-136), we obtain the action of $\overline{R}$ on any of these remaining functions $\varphi_a = R_a\Psi_0$, with $R_a \neq e$:

$$\overline{R}\varphi_a = \overline{R}R_a\Psi_0 = R_aR\Psi_0 \ . \tag{3-137}$$

Hence

$$\overline{R}\varphi_a \neq R\varphi_a(X) = RR_a\Psi_0 \ . \tag{3-138}$$

Which state should be chosen as the intrinsic state? It is clear from the above discussion that any of the g states φ_a may be chosen as the intrinsic state. However once chosen, its unique role should not be changed throughout the rest of the analysis.

In actual applications, the choice of the intrinsic state might be related to the choice of representation. For example, in the SU_3 quark model of particle physics, there are three representations, the *I-spin*, *U-spin* and *V-spin* representations (Feld 1969). The intrinsic states for these three reps are

$$\begin{aligned} &\text{(a) I-spin} \ , \quad \Psi_0(I) = |uds\rangle \ , \\ &\text{(b) U-spin} \ , \quad \Psi_0(U) = |dsu\rangle \ , \\ &\text{(c) V-spin} \ , \quad \Psi_0(V) = |sud\rangle \ , \end{aligned} \tag{3-139}$$

where u, d and s are the up, down and strange quarks, respectively. The transformations between these three reps are given in (3-226c).

Example: Let us find the effect of the intrinsic permutation $(\overline{12})$ of $\overline{S}_3$ on the six states in Table 3.6-1. The normal-ordered state $|\alpha\beta\gamma\rangle$ is chosen as the intrinsic state and the result is shown in Table 3.7.

Table 3.7. The effect of $(\overline{12})$ on the φ_i.

φ_a	$\varphi_1{=}\Phi_0$ $\lvert\alpha\beta\gamma\rangle$	$\varphi_2 = (12)\Phi_0$ $\lvert\beta\alpha\gamma\rangle$	$\varphi_3 = (13)\Phi_0$ $\lvert\gamma\beta\alpha\rangle$	$\varphi_4 = (23)\Phi_0$ $\lvert\alpha\gamma\beta\rangle$	$\varphi_5 = (123)\Phi_0$ $\lvert\gamma\alpha\beta\rangle$	$\varphi_6 = (132)\Phi_0$ $\lvert\beta\gamma\alpha\rangle$
$(\overline{12})\varphi_a$	$(12)\Phi_0$ $\lvert\beta\alpha\gamma\rangle$	Φ_0 $\lvert\alpha\beta\gamma\rangle$	$(13)(12)\Phi_0$ $\lvert\gamma\alpha\beta\rangle$	$(23)(12)\Phi_0$ $\lvert\beta\gamma\alpha\rangle$	$(123)(12)\Phi_0$ $\lvert\gamma\beta\alpha\rangle$	$(132)(12)\Phi_0$ $\lvert\alpha\gamma\beta\rangle$

One sees that acting on the product state, the intrinsic permutation $(\overline{12})$ is equivalent to the state permutation $\wp_{12} = (\alpha\beta)$. This does not occur fortuitously. We shall show in Sec. *3.7.7* that the state–permutation group $\mathcal{S}_n$ is a realization of the intrinsic permutation group $\overline{S}_n$ in the space of product states.

3.7.3. The regular representation of intrinsic groups

Equation (3-127) shows that the group space L_g forms a representation space for the intrinsic group $\bar{G}$:

$$\overline{R}_b R_c = \sum_{a=1}^{g} D_{ac}(\overline{R}_b) R_a = R_c R_b \ , \tag{3-140a}$$

Therefore

$$D_{ac}(\overline{R}_b) = \begin{cases} 1 \ , & \text{for} \quad R_c R_b = R_a \\ 0 \ , & \text{otherwise} \end{cases} \ . \tag{3-140b}$$

The rep $D(\overline{G})$ will be called the regular rep of the intrinsic group $\overline{G}$. $D(\overline{G})$ was referred to as the inverted rep of G in Boerner (1963), since $D(\overline{G})$ is anti–isomorphic to G.

Comparing (3-140b) with (2-68), one sees that in obtaining the regular reps of G and $\overline{G}$ from the group table of G, the indices c and b interchange their roles. Thus reading Table 1.2 vertically instead of horizontally, one immediately obtains the regular rep of the intrinsic permutation group $\overline{S}_3$,

$$\begin{aligned} D(\bar{e}) = \{123456\}, \ D(\overline{12}) = \{215634\}, D(\overline{13}) \ = \{361542\}, \\ D(\overline{23}) = \{456123\}, D(\overline{123}) = \{542361\}, \ D(\overline{132}) = \{634215\} \, . \end{aligned} \tag{3-141}$$

Let A be a vector in the group space L_g,

$$A = \sum_a u_a R_a \ . \tag{3-142a}$$

Its representation matrix $D_{ab}(A) = \langle a|A|b\rangle$ is determined by

$$AR_b = \sum_a \langle a|A|b\rangle R_a \ . \tag{3-142b}$$

The corresponding intrinsic element is

$$\overline{A} = \sum_a u_a \overline{R}_a \ . \tag{3-142c}$$

Its representation matrix $D_{ab}(\overline{A})$ is determined by

$$\overline{A} R_b = R_b A = \sum_a D_{ab}(\overline{A}) R_a = \sum_a \langle a|\overline{A}|b\rangle R_a \ . \tag{3-142d}$$

Theorem 3.18: The matrices $D(\overline{A})$ and $\widetilde{D}(A)$ are similar matrices, $\widetilde{D}(A)$ being the transpose of $D(A)$.

Proof: Taking the Hermitian conjugate of (3-142b), letting $A \leftrightarrow A^\dagger$, and using the unitarity of the group operators,

$$R_b^{-1} A = \sum_a \langle b|A|a\rangle R_a^{-1} \ . \tag{3-143a}$$

Comparing (3-142d) with (3-143a), we obtain

$$\langle a|\overline{A}|b\rangle = \langle b^{-1}|A|a^{-1}\rangle \ , \tag{3-143b}$$

where

$$\langle b^{-1}|A|a^{-1}\rangle = \langle R_b^{-1}|A|R_a^{-1}\rangle \ .$$

Since R_a^{-1} and R_b^{-1} are still vectors of the group space, the matrices $\langle b^{-1}|A|a^{-1}\rangle$ and $\langle b|A|a\rangle$ are similar. Thus (3-143b) shows that $D(\overline{A})$ and $\widetilde{D}(A)$ are similar matrices, that is

$$\langle a|\overline{A}|b\rangle = T\langle b^{-1}|A|a^{-1}\rangle T^{-1} \quad \text{or,}$$

$$D(\overline{A}) = T\widetilde{D}(A)T^{-1} \ . \quad \textbf{QED} \tag{3-143c}$$

Ex. 3.8. Verify that in the group space $D(C) = D(\bar{C})$, where C is the CSCO of S_3.

3.7.4. Action of intrinsic group elements on functions on the group

In analogy with (2-85) and (2-86), we can deduce from (3-127) the operation of the intrinsic group elements on functions on the group, $u(S)$. Applying $\overline{R}$ to any vector $P = \sum_S u(S)S$ in L_g gives

$$\overline{R}P = \overline{R}\sum_S u(S)S = PR = \sum_S u(S)SR = \sum_S u(SR^{-1})S \ .$$

Therefore we have

$$\overline{R}u(S) = u(SR^{-1}) \ . \tag{3-144}$$

3.7.5. Properties of the intrinsic group

1. $\overline{G}$ commutes with G, that is

$$[\overline{R}, S] = 0 \ . \tag{3-145}$$

2. $\overline{G}$ and G are anti-isomorphic.

Therefore, all the conclusions about the group G apply to the intrinsic group $\overline{G}$ as well. For example, if $C = k_1C_{i_1} + \ldots + k_lC_{i_l}$ is a CSCO of G, then $\overline{C} = k_1\overline{C}_{i_1} + \ldots + k_l\overline{C}_{i_l}$ is a CSCO of $\overline{G}, \overline{C}_i$ being the class operators of $\overline{G}$,

$$\overline{C}_i = \sum_{l=1}^{g_i} \overline{R}_l^{(i)} \ . \tag{3-146}$$

If G has N inequivalent irreps (ν), so as $\overline{G}$. If G has a subgroup chain $G \supset G_1 \supset G_2 \supset \ldots$, then $\overline{G}$ has also a subgroup chain $\overline{G} \supset \overline{G}_1 \supset \overline{G}_2 \supset \ldots$, and so on.

Theorem 3.19: The CSCO of $\overline{G}$ and G are equal:

$$\overline{C} = C \ . \tag{3-147}$$

Proof: From definition (3-127),

$$\overline{C}_iR = \Big(\sum_l \overline{R}_l^{(i)}\Big)R = R\sum_l R_l^{(i)} = RC_i \ . \tag{3-148}$$

On the other hand, the class operators of G commute with any elements of $G, RC_i = C_iR$. Hence

$$\overline{C}_iR = C_iR \ . \tag{3-149}$$

Since R is an arbitrary element, we have $\overline{C}_i = C_i$. **QED**

Because of Theorem 3.19 , if $P^{(\nu)}$ is an eigenvector of C, then it is also an eigenvector of $\overline{C}$, and if $\psi^{(\nu)}$ belongs to the irrep (ν) of G, then it must also belong to an irrep of the intrinsic group $\overline{G}$, which can be labelled by the same quantum number ν.

From (3-140a) and (3-144) one sees that the operators of the intrinsic group are unitary both in group space and in the space of functions on the group. For example, the regular rep of $\overline{S}_3$ in Eq. (3-141) is unitary.

3.7.6. Some remarks

1. From (3-127) it is seen that, for an Abelian group, the intrinsic group $\overline{G}$ coincides with the group G itself.

2. The intrinsic group element $\overline{R}$ defined by (3-127) is not a conjugate element of the group element R. From (3-127) a formal relation between $\overline{R}$ and R can be written as

$$\overline{R} = SRS^{-1} , \quad \text{when } \overline{R} \text{ acts on } S . \tag{3-150}$$

It should be stressed that the last result is not an identity either. It only shows that when acting on $S, \overline{R}$ is equivalent to the operator SRS^{-1}, and that while acting on another vector $T, \overline{R}$ will be equivalent to TRT^{-1}. In other words, the element S in Eq. (3-150) is not fixed; it changes according to which vector the operator $\overline{R}$ in acting upon. This is a most important point, albeit a little bit tricky, in understanding of the intrinsic group.

In contrast, an element T conjugate to the group element R is

$$T = S_0 R S_0^{-1} , \tag{3-151}$$

where S_0 is a fixed element of G. Equation (3-151) is an identity relation and T is an element of G.

3. One should not confuse the intrinsic group $\overline{G}$ with the group G' brought about by an inner automorphism (Sec. 1.4):

$$G' = R_a G R_a^{-1} . \tag{3-152}$$

4. It is important to distinguish between the subgroup $\overline{G}(1)$ of the intrinsic group $\overline{G}$ of G and the intrinsic group $\overline{G}'(1)$ of the subgroup $G(1)$ of G. $\overline{G}(1)$ is defined in the whole group space of G, while $\overline{G}'(1)$ is defined in the group space of $G(1)$. Let $R, R(1), \overline{R}(1)$, and $\overline{R}'(1)$ be the group elements of the groups $G, G(1), \overline{G}(1)$ and $\overline{G}'(1)$, respectively. The definition for the groups $\overline{G}(1)$ and $\overline{G}'(1)$ are, respectively,

$$\overline{R}(1)R = RR(1) \quad \text{for all } R \in G , \tag{3-153}$$

$$\overline{R}'(1)S(1) = S(1)R(1), \quad \text{for all } S(1) \in G(1) . \tag{3-154}$$

Obviously, $\overline{G}(1)$ commutes with the whole group G, while $\overline{G}'(1)$ commutes only with the subgroup $G(1)$, that is

$$[\overline{G}(1), G] = 0 , \quad [\overline{G}'(1), G] \neq 0 \quad [\overline{G}'(1), G(1)] = 0 . \tag{3-155}$$

5. The set of intrinsic operators $\{\bar{R}_a^{-1}, i = 1, 2, \cdot, g\}$ form what is called the right regular representation of G (Coleman-68).

3.7.7. Intrinsic permutation groups and state permutation groups

Theorem 3.20: With the normal order state $|\omega_0\rangle = |i_1 i_2 \ldots i_n\rangle$ as the intrinsic state, the intrinsic permutation is the inverse of the state permutation, that is

$$\overline{p} = \wp^{-1} . \tag{3-156}$$

Proof: The commutation of S_n with both $\overline{S}_n$ and $\mathcal{S}_n$, along with Eqs. (3-110) and (3-136), give

$$\overline{p}\varphi_a = \overline{p}p_a|\omega_0\rangle = p_a p|\omega_0\rangle = p_a \wp^{-1}|\omega_0\rangle = \wp^{-1} p_a|\omega_0\rangle = \wp^{-1}\varphi_a . \tag{3-157}$$

Since φ_a is an arbitrary function, (3-155) is true. **QED**

Henceforth, for the treatment of product states, we always use the state–permutation group instead of the more abstract intrinsic permutation group.

The advantage of choosing the normal-order state as the intrinsic state is that the quantum numbers of the intrinsic permutation group, which are relative to the intrinsic state, are directly related to the quantum numbers of the unitary groups (see Sec. 7.5).

Since the classes of the permutation group are all ambivalent we know from (3-156) that the class operators of S_n and $\mathcal{S}_n$, as well as their respective subgroups, S_i and $\mathcal{S}_i$, are equal. Therefore, the CSCO of S_i and $\mathcal{S}_i$ are equal,

$$\overline{C}(i) = C(i) \ , \quad i = n, n-1, \ldots, 2 \ . \tag{3-158}$$

3.8. CSCO–II and CSCO–III of G

In this section the discussion on the group S_3 is to be extended to any finite group G. We seek the eigenvectors $P^{(\nu)}$ of the CSCO of G in the group space L_g,

$$P^{(\nu)} = \sum_{a=1}^{g} u_{\nu a} R_a \ , \tag{3-159}$$

$$CP^{(\nu)} = \nu P^{(\nu)} \ . \tag{3-160}$$

Written in matrix form (3-160) becomes

$$\sum_{b=1}^{g} (C_{ab} - \nu \delta_{ab}) u_{\nu b} = 0 \ . \tag{3-161}$$

The matrix (C_{ab}) is the representative of the operator C in the regular rep:

$$CR_b = \sum_{a=1}^{a} C_{ab} R_a, \quad C_{ab} = \langle R_a | C | R_b \rangle \equiv (R_a, CR_b) \ . \tag{3-162}$$

C is a CSCO for the N–dimensional class space but is no longer a CSCO for the g–dimensional group space L_g. According to Theorem 3.11, the eigenvalues of C in L_g remain the N distinct values $\nu_1, \nu_2, \ldots, \nu_N$, determined in the class space, but each eigenvalue ν has the degeneracy $M_\nu \geq 1$. From Eqs. (3-160) and (2-37) one has

$$\det |C_{ab} - \nu \delta_{ab}|_1^g = \prod_{i=1}^{n} (\nu - \nu_i)^{M_{\nu_i}} = 0 \ , \tag{3-163}$$

$$\sum_{i=1}^{N} M_{\nu_i} = g \ . \tag{3-164a}$$

The set of eigenvectors $P^{(\nu_i)}$ of C with the same eigenvalue ν_i form a basis for an eigenspace L_{ν_i} of C, whose dimension is the degeneracy M_{ν_i}. The group space is decomposed into a direct sum of the N eigenspaces,

$$L_g = \sum_{\nu=1}^{N} \oplus L_\nu \ . \tag{3-164b}$$

To lift the degeneracy of ν entirely, we have to add extra operators to C, so that it becomes a CSCO of the g–dimensional group space L_g. These extra operators must commute with one another and with C. By virtue of Theorem 3.4, the class operators that are not included in

C are useless for lifting the degeneracy. Possible candidates for these extra operators are the CSCO of subgroups of G. Suppose that G has a subgroup chain

$$G \supset G(s) \ , \quad G(s) = G(s_1) \supset G(s_2) \supset \dots \ . \tag{3-164c}$$

We use $C(s_i)$ to designate the CSCO of the subgroup $G(s_i)$ and $C(s)$ to denote the set of operators $(C(s_1), C(s_2), \dots)$. Obviously, the operators $C(s_i)$ commute with C and with one another.

By the anti-isomorphism between G and $\overline{G}$, we have the intrinsic subgroup chain

$$\overline{G} \supset \overline{G}(s) \ , \quad \overline{G}(s) = \overline{G}(s_1) \supset \overline{G}(s_2) \supset \dots \tag{3-164d}$$

and the CSCO $\overline{C}(s) = (\overline{C}(s_1), \overline{C}(s_2), \dots)$. $\overline{C}(s)$ commutes with both C and $C(s)$, that is

$$[C(s) \ , \overline{C}(s)] = 0 \ . \tag{3-165}$$

The $\overline{C}(s)$ are also candidates for the extra operators to be added to the CSCO of G.

Definition 3.4: If, starting from the group G, we can find a group chain (3-164c) and the corresponding operator set K,

$$K = \big(C, C(s), \overline{C}(s)\big) \ , \tag{3-166a}$$

$$C(s) = \big(C(s_1), C(s_2), \dots\big) \ , \quad \overline{C}(s) = \big(\overline{C}(s_1), \overline{C}(s_2), \dots\big) \ , \tag{3-166b}$$

such that K is a CSCO for the g-dimensional group space L_g, then K is called a CSCO-III of G, while

$$M = (C, C(s)) \ , \tag{3-166c}$$

is called a CSCO-II of G.

According to the definition, in group space K has g distinct sets of eigenvalues

$$\begin{aligned} &\lambda = (\nu, m, k) \ , \\ &m = (\lambda(s_1), \lambda(s_2), \dots), \quad k = (\overline{\lambda}(s_1) \ , \overline{\lambda}(s_2), \dots) \ . \end{aligned} \tag{3-166d}$$

Theorem 3.21: If $G \supset G(s)$ is a canonical subgroup chain, then $M = (C, C(s))$ is a CSCO-II of G, and $K = (C, C(s), \overline{C}(s))$ is a CSCO-III of G.

The proof of this theorem is left to the reader as an exercise.

In many cases, the operator set K in (3-166a) is over determined in the sense that the following K may already be a CSCO in L_g:

$$\begin{aligned} &K = \big(C', C'(s), \overline{C}'(s)\big) \ , \\ &C'(s) = \big(C'(s_1), C'(s_2) \dots\big), \quad \overline{C}'(s) = \big(\overline{C}'(s_1), \overline{C}'(s_2) \dots\big) \ , \end{aligned} \tag{3-167a}$$

where C' and $C'(s_i)$ involve only some of the class operators contained in the CSCO of G and $G(s_i)$, respectively. For examples, see Ex 3.15, Ex 3.16 and Sec. 4.5.

Furthermore, in analogy with (3-35), each operator set $C'(s_i)$ can be assumed to consist of only a single operator, and we can use a single operator A and $\overline{A}$,

$$A = \sum_i d_i C'(s_i) \ , \quad \overline{A} = \sum_i d_i \overline{C}'(s_i) \tag{3-167b}$$

to replace $C'(s)$ and $\overline{C}'(s)$, where the coefficients d_i are properly chosen so that

$$K = (C', A, \overline{A}) \tag{3-167c}$$

is a CSCO in L_g. This leads to a more general definition for the CSCO–II and CSCO–III of G.

Definition 3.4′: A set of commuting operators $K = (C', A, \overline{A})$, with C' commuting with G, and A an operator set or an operator in L_g, is called a CSCO–III of G if K is a CSCO of L_g, and

$$M = (C', A) \ , \tag{3-167d}$$

is called a CSCO–II of G.

Therefore, each of the operator sets K of (3-166a), (3-167a) and (3-167c) is a possible form for the CSCO–III of G. In the following we still use $K = (C, C(s), \overline{C}(s))$ to denote a CSCO–III of G, keeping in mind that actually K could take other forms as well.

Although for an arbitrary group G, we cannot yet prove the existence of a canonical subgroup chain, for the finite groups commonly used in physics it is easy to find their canonical subgroup chains.

In practical applications, the subgroup chain $G \supset G(s)$ is often specified by the physical problem being studied (see Sec. 3.20). It may be that the physically required subgroup chain $G \supset G(s)$ is not a canonical one. In such a case, $(C, C(s), \overline{C}(s))$ is not a CSCO in L_g, and thus is not a CSCO-III of G.

According to Dirac (1958, Sec. 14), any set of commuting operators can be made into a complete set of commuting operators by adding certain operators to it. Let us first add one operator ξ. This operator can always be written as a linear combination of the g group operators, $\xi = \sum_a \xi_a R_a$, where the ξ_a are complex numbers, since we are working in the group space L_g. Corresponding to the operator ξ, there is the intrinsic operator $\overline{\xi} = \sum_a \xi_a \overline{R}_a$. Thus the additional operators always occur in pairs. If $\left(C, C(s), \xi, \overline{C}(s), \overline{\xi}\right)$ is not yet a CSCO of L_g, we can add another pair of operators η and $\overline{\eta}$, and so on until

$$\left(C, C''(s), \overline{C}''(s)\right) \tag{3-168a}$$

is a CSCO of L_g, where

$$C''(s) = \left(C(s), \xi, \eta, \dots\right) \ , \qquad \overline{C}''(s) = \left(\overline{C}(s), \overline{\xi}, \overline{\eta}, \dots\right) \ . \tag{3-168b}$$

Hence we can always find a CSCO–III of G regardless of whether $G \supset G(s)$ is canonical or not. To be specific, in the following we shall assume that $G \supset G(s)$ is a canonical subgroup chain unless otherwise stated. For the non–canonical case, all we need to do is to reinterpret the meaning of $C(s)$ and $\overline{C}(s)$ in accordance with (3-168a).

We can also choose a single operator

$$K = C + \sum_i [\alpha_i C(s_i) + \beta_i \overline{C}(s_i)] \ , \tag{3-168c}$$

as a CSCO–III of G, where the coefficients α_i and β_i are properly chosen so that K has g distinct eigenvalues.

3.9. Full Reduction of the Regular Representation

3.9.1. Eigenvectors of the CSCO–III *of G*

Let $P_m^{(\nu)k}$ be the eigenvectors of the CSCO–III of G in the group space L_g,

$$\begin{pmatrix} C \\ C(s) \\ \overline{C}(s) \end{pmatrix} P_m^{(\nu)k} = \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} P_m^{(\nu)k}, \quad P_m^{(\nu)k} = \sum_{a=1}^{g} u_{\nu mk,a} R_a \ . \tag{3-169a}$$

There is a one–to–one correspondence between $P_m^{(\nu)k}$ and the vector $\mathbf{u}_{\nu mk}$ defined as

$$\mathbf{u}_{\nu mk} = (u_{\nu mk,1}, \dots, u_{\nu mk,g}) \ .$$

Using $\overline{R}S = SR$, we can rewrite the third equation in (3-169a) as

$$\overline{C}(s)P_m^{(\nu)k} = P_m^{(\nu)k}C(s) = kP_m^{(\nu)k} , \tag{3-169b}$$

where $m(k)$ denotes the set of eigenvalues (3-166d) if $C(s)[\overline{C}(s)]$ is interpreted as in (3-166b), or simply the eigenvalue of $A(\overline{A})$, if $C(s)[\overline{C}(s)]$ is interpreted as $A(\overline{A})$. To be specific we assume, in the following, that

$$C(s) = A , \quad \overline{C}(s) = \overline{A} . \tag{3-169c}$$

Theorem 3.22 The representatives of the operators A and $\overline{A}$ in the eigenspace L_ν of C are similar matrices.

Proof: Let the M_ν basis vectors in L_ν be

$$\varphi_i = \sum_a v_{ia}R_a , \quad i = 1, 2, \ldots, M_\nu , \tag{3-170a}$$

$$C\varphi_i = \nu\varphi_i . \tag{3-170b}$$

One obtains, using Eq. (3-137f) in the second equality

$$\langle\varphi_i|\overline{A}|\varphi_j\rangle = \sum_{ab}\langle v_{ia}R_a|\overline{A}|v_{jb}R_b\rangle = \sum_{ab} v_{ia}^* v_{jb}\langle R_b^{-1}|A|R_a^{-1}\rangle = \langle\varphi_j'|A|\varphi_i'\rangle , \tag{3-170c}$$

where

$$\varphi_i' = \sum_a v_{ia}^* R_a^{-1} .$$

Taking the Hermitian conjugate of (3-170b), and using the self–adjointness of C and the unitarity of R_a, one has

$$C\varphi_i' = \nu\varphi_i' . \tag{3-171}$$

This shows that $\varphi_i' \in L_\nu$. Thus φ_i' is necessarily a linear combination of the M_ν basis vectors φ_i. Therefore (3-170c) tells us that the representative matrices of A and $\overline{A}$ in L_ν are similar, that is, $\mathcal{D}^{(\nu)}(A) \sim \mathcal{D}^{(\nu)}(\overline{A})$. **QED**

Suppose that $\mathcal{D}^{(\nu)}(A)$ has $|\nu|$ distinct eigenvalues $m_1, \ldots, m_{|\nu|}$, while $\mathcal{D}^{(\nu)}(\overline{A})$ has $|\overline{\nu}|$ distinct eigenvalues $k_1, \ldots, k_{|\overline{\nu}|}$. Since $(C, \overline{A})$ commutes with the group G, its eigenspace $L_{(\nu)k} = \{P_{m_i}^{(\nu)k} : i = 1, 2, \ldots, |\nu|\}$ is necessarily a rep space of G and the degeneracy of m_i is necessarily independent of i, as mentioned in Sec. 3.3.3.

Furthermore, according to the hypothesis that $(C, A, \overline{A})$ is a CSCO of L_g, $(A, \overline{A})$ is necessarily a CSCO in each eigenspace $L_\nu, \nu = 1, 2, \ldots, N$. Therefore the degeneracy of m_i in L_ν is totally eliminated by the eigenvalues of $\overline{A}$. In other words the degeneracy of m_i must be equal to the number $|\overline{\nu}|$ of the distinct eigenvalues of $\overline{A}$. Therefore, the characteristic equation for $\mathcal{D}^{(\nu)}(A)$ has the form

$$\det|\mathcal{D}^{(\nu)}(A) - m \cdot I| = \prod_{i=1}^{|\nu|}(m - m_i)^{|\overline{\nu}|} . \tag{3-172a}$$

Similarly, interchanging G and $\overline{G}$, we have

$$\det|\mathcal{D}^{(\nu)}(\overline{A}) - k \cdot I| = \prod_{i=1}^{|\overline{\nu}|}(k - k_i)^{|\nu|} . \tag{3-172b}$$

Since, by Theorem 3.22 , $\mathcal{D}^{(\nu)}(A)$ and $\mathcal{D}^{(\nu)}(\overline{A})$ have identical characteristic equations, we have that

$$|\nu| = |\overline{\nu}| = h_\nu , \quad m_i = k_i, \quad i = 1, 2, \ldots, h_\nu . \tag{3-172c}$$

In the following, $m(k)$ is also used as an index to enumerate the eigenvalues, and thus we can write $m, k = 1, 2, \ldots, h_\nu$.

The conservation of dimension in (3-172a) or (3-172b) gives

$$h_\nu^2 = M_\nu \ , \tag{3-172d}$$

which we formalize as Theorem 3.23 .

Theorem 3.23: The dimension of the eigenspace L_ν of C is necessarily a square of an integer.

Stated differently, the number of distinct sets of eigenvalues (m, k) of $(A, \overline{A})$ in L_ν has to be equal to the dimension of L_ν.

From Eqs. (3-164a) and (3-172d) we get

$$g = \sum_{i=1}^{N} h_{\nu_i}^2 \ . \tag{3-173}$$

Now the eigenspace L_ν of C is further decomposed into h_ν rep spaces of G,

$$L_\nu = \sum_{k=1}^{h_\nu} \oplus L_{(\nu)k} \ , \quad L_{(\nu)k} = \{P_m^{(\nu)k} : m = 1, 2, \ldots, h_\nu\} \ . \tag{3-174}$$

Analogously, since $(C, C(s))$ commutes with $\overline{G}$, which is the eigenspace of $(C, C(s))$,

$$\overline{L}_{(\nu)m} = \{P_m^{(\nu)k} : k = 1, 2, \ldots, h_\nu\} \ , \tag{3-174'}$$

is a rep space of the intrinsic group $\overline{G}$. Hence, the space L_ν can also be decomposed into h_ν rep spaces $\overline{L}_{(\nu)m}$ of $\overline{G}$,

$$L_\nu = \sum_{m=1}^{h_\nu} \oplus \overline{L}_{(\nu)m} \ . \tag{3-175}$$

The eigenequation (3-169a) can be written in matrix form as

$$\sum_{b=1}^{g} \left[\left\langle a \left| \begin{matrix} C \\ C(s) \\ \overline{C}(s) \end{matrix} \right| b \right\rangle - \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} \delta_{ab} \right] u_{\nu mk,b} = 0 \ , \tag{3-176}$$

where $\langle a|C|b\rangle = (R_a, CR_b) = C_{ab}$, and

$$C(s)R_b = \sum_a \langle a|C(s)|b\rangle R_a \ , \tag{3-177}$$

$$\overline{C}(s)R_b = R_b C(s) = \sum_a \langle a|\overline{C}(s)|b\rangle R_a \ . \tag{3-178}$$

The eigenvectors of the CSCO–III form an orthonormal and complete set in the group space L_g,

$$\langle P_m^{(\nu)k} | P_{m'}^{(\nu')k'} \rangle = \delta_{\nu\nu'}\delta_{mm'}\delta_{kk'} \ , \tag{3-179a}$$

$$\sum_{\nu mk} |P_m^{(\nu)k}\rangle\langle P_m^{(\nu)k}| = 1 \ . \tag{3-179b}$$

Using (3-169a), (3-179) becomes

$$\sum_a u_{\nu mk,a}^* u_{\nu' m' k',a} = \delta_{\nu\nu'}\delta_{mm'}\delta_{kk'} \ , \tag{3-180a}$$

$$\sum_{\nu mk} u^*_{\nu mk,a} u_{\nu mk,b} = \delta_{ab} \ . \tag{3-180b}$$

With the help of the last result, the inverse expansion to (3-169a) is

$$R_a = \sum_{\mu ji} u^*_{\mu ji,a} P_j^{(\mu)i} \ . \tag{3-181}$$

3.9.2. The representations $D^{(\nu)k}(G)$ and $D^{(\nu)m}(\overline{G})$

Since C commutes with the group elements and in turn with $P_m^{(\nu)k}$,

$$C P_j^{(\mu)i} P_m^{(\nu)k} = \mu P_j^{(\mu)i} P_m^{(\nu)k} = \nu P_j^{(\mu)i} P_m^{(\nu)k} \ . \tag{3-182}$$

Therefore

$$(\nu - \mu) P_j^{(\mu)i} P_m^{(\nu)k} = 0 \ . \tag{3-183}$$

From (3-169a) and (3-129), it follows that

$$C(s)(P_j^{(\mu)i} P_m^{(\nu)k}) = j(P_j^{(\mu)i} P_m^{(\nu)k}) \ , \tag{3-184}$$

$$\overline{C}(s)(P_j^{(\mu)i} P_m^{(\nu)k}) = (P_j^{(\mu)i} P_m^{(\nu)k})\overline{C}(s) = k(P_j^{(\mu)i} P_m^{(\nu)k}) \ . \tag{3-185}$$

Furthermore it follows from (3-169b) that

$$P_j^{(\mu)i} C(s) P_m^{(\nu)k} = \begin{cases} P_j^{(\mu)i}\big(C(s) P_m^{(\nu)k}\big) = m P_j^{(\mu)i} P_m^{(\nu)k} \ . \\ \big(P_j^{(\mu)i} C(s)\big) P_m^{(\nu)k} = i P_j^{(\mu)i} P_m^{(\nu)k} \ . \end{cases}$$

Thus

$$(m - i) P_j^{(\mu)i} P_m^{(\nu)k} = 0 \ . \tag{3-186}$$

Due to the non-degeneracy of the eigenvalues of the CSCO-III, the above results imply that

$$P_j^{(\mu)i} P_m^{(\nu)k} = \delta_{\nu\mu} \delta_{im} \xi_{jm}^{(\nu)k} P_j^{(\nu)k} \ , \tag{3-187}$$

where $\xi_{jm}^{(\nu)k}$ is a constant to be decided upon.

Applying R_a of (3-181) to $P_m^{(\nu)k}$ and using Eq. (3-187), one gets

$$R_a P_m^{(\nu)k} = \sum_j D_{jm}^{(\nu)k}(R_a) P_j^{(\nu)k} \ , \tag{3-188a}$$

where

$$D_{jm}^{(\nu)k}(R_a) = \langle P_j^{(\nu)k} | R_a | P_m^{(\nu)k} \rangle = \xi_{jm}^{(\nu)k} u^*_{\nu jm,a} \ . \tag{3-188b}$$

Thus the eigenvectors $P_m^{(\nu)k} (m = 1, 2, \ldots, h_\nu)$ form the basis of the k-th rep (ν) of the group G with the rep matrices $D^{(\nu)k}(R_a), k = 1, 2, \ldots, h_\nu$.

Similarly for the group $\overline{G}$, we have

$$\overline{R}_a P_j^{(\nu)k} = P_j^{(\nu)k} R_a = \sum_i D_{ik}^{(\nu)j}(\overline{R}_a) P_j^{(\nu)i} \ , \tag{3-189a}$$

$$D_{ik}^{(\nu)j}(\overline{R}_a) = \langle P_j^{(\nu)i} | \overline{R}_a | P_j^{(\nu)k} \rangle = \xi_{jk}^{(\nu)i} u^*_{\nu ki,a} \ . \tag{3-189b}$$

These show that the eigenvectors $P_m^{(\nu)k} (k = 1, 2, \ldots, h_\nu)$ form the basis of the m-th rep (ν) of the intrinsic group $\overline{G}$ with the rep matrices $D^{(\nu)m}(\overline{R}_a)$, $m = 1, 2, \ldots h_\nu$.

Ex. 3.9. Check that in the eigenspace $L_{(0)}$ of the CSCO of S_3, $\mathcal{D}^{(0)}$ (12) and $\mathcal{D}^{(0)}(\overline{12})$ are similar matrices, where $L_{(0)} = \{\mathbf{1-6}, \mathbf{5-6}, \mathbf{2-3}, \mathbf{3-4}\}$, the boldface integers being shorthand

notation for the group elements.

3.9.3. The standard phase choice for $\mathbf{u}_{\nu mk}$

The eigenvector $\mathbf{u}_{\nu jm}$ in (3-169a) is determined up to a phase factor. We shall now show that the phase can be chosen to simplify the relation between the eigenvectors $\mathbf{u}_{\nu jm}$ and the matrix elements of the rep matrices $D^{(\nu)}_{jm}$.

Letting $R_a = e$ in (3-188b), we get

$$\delta_{jm} = \xi^{(\nu)k}_{mj} u^*_{\nu jm,e} \ . \tag{3-190a}$$

Hence $\xi^{(\nu)k}_{mm}$ must be independent of k. Letting $\overline{R}_a = e$ in (3-189b), we get

$$\delta_{ik} = \xi^{(\nu)i}_{jk} u^*_{\nu ki,e} \ . \tag{3-190b}$$

Hence $\xi^{(\nu)k}_{jk}$ must be independent of j. Both equations (3-190a) and (3-190b) are independent of phase choices.

Let us now choose phases such that the rep matrices $D^{(\nu)k}(R_a)$ are independent of k. From (3-188b), this is equivalent to the choice that $\xi^{(\nu)k}_{jm}$ is independent of k. One of these coefficients $\xi^{(\nu)k=m}_{jm}$ has already been shown by (3-190b) to be independent of j. By choosing $\xi^{(\nu)k}_{jm}$ to be independent of k, we have extended the j independence from the diagonal case $k = m$ to the general case of any k. Hence all coefficients $\xi^{(\nu)k}_{jm}$ are independent of both j and k. This means that the rep matrices $D^{(\nu)j}(\overline{R}_a)$ are independent of j.

The coefficients $\xi^{(\nu)k}_{jm}$ can now be denoted more simply as $\xi^{(\nu)}_m$. Similarly (3-188b) simplifies to

$$D^{(\nu)}_{jm}(R_a) = \xi^{(\nu)}_m u^*_{\nu jm,a} \ . \tag{3-191}$$

Equations (3-180a) and (3-191) now give

$$\sum_{a=1}^{g} |D^{(\nu)}_{jm}(R_a)|^2 = |\xi^{(\nu)}_m|^2 \ . \tag{3-192}$$

Summing over the index j from 1 to h_ν, and using the unitarity of the rep matrix $D^{(\nu)}$, we obtain

$$g = |\xi^{(\nu)}_m|^2 h_\nu \ . \tag{3-193}$$

This shows that $\xi^{(\nu)}_m$ has the amplitude–phase representation $\xi^\nu \eta_m$ with the m–independent amplitude

$$\xi^\nu = (g/h_\nu)^{\frac{1}{2}} \ . \tag{3-194}$$

Only the phase factor η_m depends on m. From (3-190a), which now reads

$$1 = \xi^\nu \eta_m u^*_{\nu mm,e} \ , \tag{3-195a}$$

we see that η_m is also the phase factor for $u_{\nu mm,e}$.

We now make the final phase choice that removes the remaining m dependence, namely that

$$\eta_m = 1 \ . \tag{3-195b}$$

With this phase choice, both ξ^ν and $u_{\nu mm,e}$ are real and positive. This phase choice shall be referred to as the *standard phase choice* in the EFM.

With this standard phase choice, Eq. (3-187) becomes

$$P_j^{(\nu)i} P_m^{(\nu)k} = \sqrt{\frac{g}{h_\nu}} \delta_{\nu\mu} \delta_{im} P_j^{(\nu)k} \ , \tag{3-196}$$

equations (3-188), (3-189) and (3-169a) reduce to

$$R P_m^{(\nu)k} = \sum_{m'} D^{(\nu)}_{m'm}(R) P_{m'}^{(\nu)k} \quad k = m_1, m_2, \ldots, m_{h_\nu}, \tag{3-197a}$$

$$\overline{R} P_m^{(\nu)k} = P_m^{(\nu)k} R = \sum_{k'} D^{(\nu)}_{k'k}(\bar{R}) P_m^{(\nu)k'}, \ m = m_1, m_2, \ldots, m_{h_\nu} \ , \tag{3-197b}$$

$$D^{(\nu)}_{mk}(R_a) = D^{(\nu)}_{km}(\overline{R}_a) = \sqrt{\frac{g}{h_\nu}} u^*_{\nu mk,a} \ , \tag{3-198}$$

$$P_m^{(\nu)k} = \sqrt{\frac{h_\nu}{g}} \sum_a D^{(\nu)*}_{mk}(R_a) R_a \ , \tag{3-199}$$

while Eq. (3-180) becomes

$$\frac{h_\nu}{g} \sum_{a=1}^{g} D^{(\nu)*}_{mk}(R_a) D^{(\nu')}_{m'k'}(R_a) = \delta_{\nu\nu'} \delta_{mm'} \delta_{kk'} \ , \tag{3-200a}$$

$$\sum_{\nu=1}^{N} \sum_{m,k=1}^{h_\nu} \frac{h_\nu}{g} D^{(\nu)*}_{mk}(R_a) D^{(\nu)}_{mk}(R_b) = \delta_{ab} \ . \tag{3-200b}$$

As will be shown shortly, the rep $D^{(\nu)}$ is irreducible, and Eq. (3-200) are the two *orthogonality theorems* for the irreducible matrix elements

From the above discussion, we see that the standard phase choice can be realized as follows:

1. By virtue of (3-195) (which now reads $\xi^\nu u^*_{\nu mm,e} = 1$), the coefficients $u_{\nu mm,e}$, $m = 1, 2, \ldots, h_\nu$, should be real and positive.

2. For each irrep ν of G, the overall phases of the eigenvectors for a particular k, say the first one, $\mathbf{u}_{\nu mk=1}, m = 2, 3, \ldots, h_\nu$, can be chosen arbitrarily, or with the help of a suitable phase convention.

3. By virtue of (3-198), the phase of the eigenvector $\mathbf{u}_{\nu mk}$ for $k \neq 1$ should be fixed by requiring that a nonzero coefficient $u_{\nu mk,a}$ in (3-169a) in front of a suitable group element R_a be equal to

$$D^{(\nu)}_{mk}(R_a)^* = (h_\nu/g)^{\frac{1}{2}} \langle P_m^{(\nu)1} | R_a | P_k^{(\nu)1} \rangle^* \ , \tag{3-201}$$

as calculated from the eigenvectors $\mathbf{u}_{\nu mk=1}$ with chosen phases. The matrix element (3-201) can be obtained with the help of the group table.

Under the standard phase choice the h_ν reps, $D^{(\nu)k}(G), k = 1, 2, \ldots, h_\nu$, are identical, the h_ν reps $D^{(\nu)m}(\overline{G}), m = 1, 2, \ldots, h_\nu$ are identical, and $D^{(\nu)}(\overline{G}) = \widetilde{D}^{(\nu)}(G)$. Hence we have the following theorem:

Theorem 3.24: The reps $D^{(\nu)k}(G)$ $[D^{(\nu)m}(\overline{G})]$ with the same eigenvalue ν of the CSCO of G are equivalent and can be made identical to one another by using the standard phase choice.

3.9.4. The irreducibility of $D^{(\nu)}(G)$

Theorem 3.25 : The N inequivalent reps $D^{(\nu)}(G)$ resulting from the decomposition of the group space L_g of G are irreducible.

Proof: Suppose that an $h_\nu \times h_\nu$ matrix A satisfies

$$A D^{(\nu)}(R_a) = D^{(\nu)}(R_a) A \ , \quad a = 1, 2, \ldots, g \ , \tag{3-202}$$

or

$$\sum_{m'} A_{mm'} D^{(\nu)}_{m'k}(R_a) = \sum_{m'} D^{(\nu)}_{mm'}(R_a) A_{m'k} \ . \tag{3-203}$$

Multiplying both sides of (3-203) by $(h_\nu/g)D^{(\nu)*}_{ik}(R_a)$, and summing over a, from (3-200a) we obtain

$$A_{mi} = \delta_{mi} A_{kk} \ . \tag{3-204}$$

This shows that any matrix which commutes with all the matrices of the rep $D^{(\nu)}$ is a multiple of the unit matrix. According to Schur's lemma 1', $D^{(\nu)}(G)$ is irreducible. Similarly, the reps $D^{(\nu)}(\overline{G})$ for the intrinsic group are also irreducible. **QED**

Now we can give an alternative definition for the CSCO–II of G .

Definition 3.5: If all the eigenspaces of $(\overline{C}, \overline{C}(s))$ are irreducible spaces of G, then $(\overline{C}, \overline{C}(s))$ is called a CSCO–II of the intrinsic group $\overline{G}$, while the corresponding operator $(C, C(s))$, the CSCO–II of G.

Therefore, the question raised at the beginning of Chapter 3 is answered. The operator set sought after, whose eigenspaces are irreducible spaces of G, is the CSCO–II, $(\overline{C}, \overline{C}(s))$, of the intrinsic group $\overline{G}$. Recall that the CSCO–II of a group G is a CSCO in any multiplicity–free rep space of G.

One of the advantages of the EFM for constructing the irreducible basis or irreps of a group G is that the subgroup chain $G(s)$ used to classify the irreducible basis or irrep can be chosen at will without the restriction that the subgroup has to be an invariant subgroup of G.

However, if, for some circumstances, we are only interested in obtaining the irreducible basis without the requirement that it be in a certain classification scheme, then we pay attention only to the operator set $C(s)$, without bothering about its related subgroup chain. In such cases, the eigenvalue of $C(s)$ is merely used to distinguish between the components of an irreducible basis, and $C(s)$ can be chosen differently for different irreps. The choice of $C(s)$ can be arbitrary so long as its eigenvalues can provide enough labels for the basis vectors of the same irrep. For example, for two–dimensional irreps of the point or space groups, the possible choice of $C(s)$ is a (plane) reflection operator, or a two–fold rotation C_2; for irreps with $h_\nu = 3(4)$, it is a three–fold (four–fold) rotation $C_3(C_4)$.

From (3-173), we have Theorem 3.26 (Burnside's Theorem).

Theorem 3.26: The regular rep of G contains N inequivalent irreps $D^{(\nu)}, N$ being the number of classes of G; the number of times each irrep occurs is equal to its dimension.

For example, for the permutation group $S_3, g = 6, N = 3$. There are three inequivalent irreps $\nu = 3$, 0, and -3, with dimensions 1,2, and 1, respectively, $6{=}1{+}2^2{+}1$. For a non–Abelian abstract group of order eight, the only way to fulfill (3-173) is with $8{=}1{+}1{+}1{+}1{+}2^2$, since it must have the one–dimensional identity rep. Therefore, it has four one–dimensional and one two–dimensional inequivalent irreps.

The eigenvectors $P^{(\nu)k}_m$ are the $G \supset G(s)$ and $\overline{G} \supset \overline{G}(s)$ irreducible basis vectors. With regard to the group G, the external quantum number m is the component index and the intrinsic quantum number k is the *multiplicity label.* If m and k are interpreted as in (3-166d), then $P^{(\nu)k}_m$ belongs to the irreps $\nu, \lambda(s_1), \lambda(s_2), \ldots$ of $G \supset G(s_1) \supset G(s_2) \supset \ldots$, and belongs to the irreps $\nu, \overline{\lambda}(s_1), \overline{\lambda}(s_2), \ldots$ of $\overline{G} \supset \overline{G}(s_1) \supset \overline{G}(s_2) \supset \ldots$. Equation (3-197) shows that under the action of $R(\overline{R}), P^{(\nu)k}_m$ only changes its external (intrinsic) quantum number $m(k)$.

3.9.5. The EFM for $G \supset G(s)$ irreducible matrices

According to (3-198), once the eigenvectors of the CSCO–III of G have been computed, the irreducible matrices for the $G \supset G(s)$ basis, referred to as the $G \supset G(s)$ irreducible matrices,

can be readily obtained. It should be stressed that (3-198) *holds only for the standard phase choice.*

Theorem 3.27: Regarded as functions on the group, the complex conjugate of the $G \supset G(s)$ irreducible matrix elements are eigenfunctions of the CSCO–III of G,

$$\begin{pmatrix} C \\ C(s) \\ \overline{C}(s) \end{pmatrix} D^{(\nu)*}_{mk}(R_a) = \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} D^{(\nu)*}_{mk}(R_a) \ . \tag{3-205}$$

Proof: It suffices to prove that, regarded as functions on the group, $D^{(\nu)}_{mk}(R_a)^*$ is the $G \supset G(s)$ irreducible basis vector (ν, m) and the $\overline{G} \supset \overline{G}(s)$ irreducible basis vector (ν, k).

Using (2-87a) and (2-45a), one has

$$RD^{(\nu)*}_{mk}(R_a) = D^{(\nu)*}_{mk}(R^{-1}R_a) = \sum_{m'} D^{(\nu)*}_{mm'}(R^{-1}) D^{(\nu)*}_{m'k}(R_a) \ . \tag{3-206}$$

Thus, since we have a unitary irrep,

$$RD^{(\nu)*}_{mk}(R_a) = \sum_{m'} D^{(\nu)}_{m'm}(R) D^{(\nu)*}_{m'k}(R_a) \ . \tag{3-207}$$

Similarly, from (3-144) and (2-45a), we have

$$\overline{R}D^{(\nu)*}_{mk}(R_a) = D^{(\nu)*}_{mk}(R_aR^{-1}) = \sum_{k'} D^{(\nu)}_{kk'}(R) D^{(\nu)*}_{mk'}(R_a) \ . \tag{3-208}$$

Comparing (3-207) and (3-208) with (3-197a) and (3-197b) respectively, we see that $D^{(\nu)}_{mk}(R_a)^*$ is indeed the $G \supset G(s)$ and $\overline{G} \supset \overline{G}(s)$ irreducible basis. **QED**

Therefore, in the space of functions on the group, the eigenfunctions of the CSCO–III of G, the $G \supset G(s)$ and $\overline{G} \supset \overline{G}(s)$ irreducible basis, and the complex conjugate of the $G \supset G(s)$ irreducible matrix elements, are all different names for the same thing.

To simplify our notation, let us assume that $G(s) = G_f \supset G_{f-1} \supset \ldots \supset G_1$, with the CSCO $C(s) = (C(f), C(f-1), \ldots, C(1))$ and the eigenvalue $m = (\lambda_f, \lambda_{f-1}, \ldots \lambda_1)$. From

$$[C(j), R_i] = 0, \quad j = f, f-1, \ldots, i, \quad R_i \in G_i \ , \tag{3-209}$$

we know that when acting upon $P^{(\nu)k}_m$, the elements R_i of the subgroup G_i cannot change the eigenvalues $\lambda_f, \lambda_{f-1}, \ldots, \lambda_i$. Therefore

$$D^{(\nu)}_{m'm}(R_i) = \langle P^{(\nu)k}_{m'} | R_i | P^{(\nu)k}_m \rangle = \delta_{\lambda'_f \lambda_f} \ldots \delta_{\lambda'_i \lambda_i} D^{\lambda_i}_{\overline{m}'\overline{m}}(R_i) \ , \tag{3-210}$$

where $D^{\lambda_i}_{\overline{m}'\overline{m}}(R_i)$ are the matrix elements for the irrep (λ_i) of the subgroup G_i,

$$D^{(\lambda_i)}_{\overline{m}'\overline{m}}(R_i) = \langle P^{(\lambda_i)\bar{k}}_{\overline{m}'} | R_i | P^{(\lambda_i)\bar{k}}_{\overline{m}} \rangle \ . \tag{3-211}$$

Equation (3-210) shows that the $G \supset G(s)$ irreducible matrices have the nice property that they are block–diagonal for the elements belonging to any subgroup contained in the subgroup chain $G(s)$ of G.

3.9.6. Reduction of the regular representation in configuration space

We can also carry out the reduction of the regular rep in configuration space. The procedure is exactly the same as in the group space. We only need to make the following substitutions $R_a \to \varphi_a, P^{(\nu)k}_m \to \psi^{(\nu)k}_m$. Correspondingly, we have the following equations:

$$\begin{pmatrix} C \\ C(s) \\ \overline{C}(s) \end{pmatrix} \psi^{(\nu)k}_m = \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} \psi^{(\nu)k}_m \ , \tag{3-212}$$

$$\psi_m^{(\nu)k} = \sum_{a=1}^{g} u_{\nu mk,a}\varphi_a(X) = \sqrt{\frac{h_\nu}{g}} \sum_{a=1}^{g} D_{mk}^{(\nu)*}(R_a)\varphi_a(X) \ . \tag{3-213}$$

$$R\psi_m^{(\nu)k} = \sum_{m'} D_{m'm}^{(\nu)}(R)\psi_{m'}^{(\nu)k} \ , \tag{3-214}$$

$$\overline{R}\psi_m^{(\nu)k} = \sum_{k'} D_{kk'}^{(\nu)}(R)\psi_m^{(\nu)k'} \tag{3-215}$$

$$\langle\psi_m^{(\nu)k}|\psi_{m'}^{(\nu')k'}\rangle = \delta_{\nu\nu'}\delta_{mm'}\delta_{kk'}, \tag{3-216}$$

$$\sum_{\nu mk} |\psi_m^{(\nu)k}\rangle\langle\psi_m^{(\nu)k}| = 1 \ . \tag{3-217}$$

The only case which merits special consideration is that when the g basis functions φ_a are non–orthogonal, to be discussed in Sec. 3.14.

To further elucidate the transformation property of $\psi_m^{(\nu)k}$ under the group G and $\overline{G}$, we construct the following array $\Psi^{(\nu)}$ out of the h_ν^2 functions $\psi_m^{(\nu)k}$ belonging to the irrep (ν)

$$\Psi^{(\nu)} = \begin{pmatrix} \psi_1^{(\nu)1} & \psi_1^{(\nu)2} & \cdots & \psi_1^{(\nu)h_\nu} \\ \psi_2^{(\nu)1} & \psi_2^{(\nu)2} & \cdots & \psi_2^{(\nu)h_\nu} \\ \vdots & \vdots & & \vdots \\ \psi_{h_\nu}^{(\nu)1} & \psi_{h_\nu}^{(\nu)2} & \cdots & \psi_{h_\nu}^{(\nu)h_\nu} \end{pmatrix} \ . \tag{3-218}$$

Equation (3-214) [(3-215)] tells us that under the operation $R_a(\overline{R}_a)$, each column (row) in (3-218) transforms according to the same irrep $D^{(\nu)}(\tilde{D}^{(\nu)})$.

3.9.7. Example: the group S_3

In Eq. (3-119), we gave the eigenvectors $\psi_m^{(\nu)k}$, or equivalently, $P_m^{(\nu)k}$, of the CSCO–III of the permutation group S_3, but we evaded the phase problem. We now follow the three steps of subsection 3.9.3 to determine the phases of the eigenvectors. First we extract the factor $\sqrt{h_\nu/g}$ out of the coefficients $u_{\nu mk,a}$. Then the results obtained from Eq. (3-119) are as shown in Table 3.9. The phases for $\psi_m^{(\nu)m}, (\nu,m) = (3,1), (-3,-1), (0,1)$ and $(0,-1)$ are fixed by the first step.

The phase of $\psi_{-1}^{(0)1}$ can be chosen freely. Suppose it has been chosen as shown in the fourth row of Table 3.9. To determine the phase of $\psi_1^{(0)-1}$, that is the fifth row vector in Table 3.9, we need to calculate a non–vanishing matrix element $D_{1-1}^{(0)}(R_a)$ from the known irreducible basis $\psi_m^{(0)1}$, where R_a can be chosen arbitrarily; for example, we might choose $R_a = R_3 = (13)$. From the third and fourth rows of Table 3.9 and using Table 1.2 we can calculate

$$\begin{aligned} D_{1-1}^{(0)}(R_3)^* &= \langle\psi_1^{(0)1}|(13)|\psi_{-1}^{(0)1}\rangle^* \\ &= \frac{1}{\sqrt{48}}\langle 2(\mathbf{1+2}) - \mathbf{3} - \mathbf{4} - \mathbf{5} - \mathbf{6}|\mathbf{3}| - \mathbf{3} + \mathbf{4} - \mathbf{5} + \mathbf{6}\rangle \\ &= \frac{1}{\sqrt{48}}\langle 2(\mathbf{1+2}) - \mathbf{3} - \mathbf{4} - \mathbf{5} - \mathbf{6}| - \mathbf{1} + \mathbf{6} - \mathbf{2} + \mathbf{4}\rangle = -\sqrt{3}/2, \end{aligned} \tag{3-219}$$

where the boldfaced integers are shorthand notation for φ_a or R_a. The phase of $\varphi_1^{(0)-1}$ is now determined by requiring that its coefficient u_3 has the same sign as that of $D_{1-1}^{(0)}(R_3)^* = -\sqrt{3}/2$. Having adjusted the phase we can use (3-198) to read off all the irreps of S_3 from Table 3.9. For a given permutation one simply reads down the column of the table associated with that permutation. The result is identical to (3-91).

Table 3.9. The standard basis $\psi_m^{(\nu)k}(P_m^{(\nu)k})$ of S_3 and $\overline{S}_3$, with standard matrix elements.

$[D_{mk}^{(\nu)}(R_a)]$ Φ_0 / R_a / $\lambda_3,\lambda_2,\overline{\lambda}_2$ / ν,m,k	Y_m	W_k	Norm $\sqrt{\frac{h_\nu}{6}}$	$\lvert\alpha\beta\gamma\rangle$ e	$\lvert\beta\alpha\gamma\rangle$ (12)	$\lvert\gamma\beta\alpha\rangle$ (13)	$\lvert\alpha\gamma\beta\rangle$ (23)	$\lvert\gamma\alpha\beta\rangle$ (123)	$\lvert\beta\gamma\alpha\rangle$ (132)	Irreducible matrix $D_{ij}^{(\nu)}(R_a)$
$3,1,1$	$\boxed{1}\boxed{2}\boxed{3}$	$\boxed{\alpha}\boxed{\beta}\boxed{\gamma}$	$\frac{1}{\sqrt{6}}$	1	1	1	1	1	1	$D_{11}^{(3)*}$
$-3,-1,-1$	$\begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\hline\end{array}$	$\begin{array}{|c|}\hline \alpha\\\hline \beta\\\hline \gamma\\\hline\end{array}$	$\frac{1}{\sqrt{6}}$	1	-1	-1	-1	1	1	$D_{11}^{(-3)*}$
$0,1,1$	$\begin{array}{\|c\|c\|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|}\hline \alpha&\beta\\\hline \gamma\\\cline{1-1}\end{array}$	$\frac{1}{\sqrt{3}}$	1	1	$-1\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$D_{11}^{(0)*}$
$0,-1,1$	$\begin{array}{\|c\|c\|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|}\hline \alpha&\beta\\\hline \gamma\\\cline{1-1}\end{array}$	$\frac{1}{\sqrt{3}}$	0	0	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$D_{21}^{(0)*}$
$0,1,-1$	$\begin{array}{\|c\|c\|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|}\hline \alpha&\gamma\\\hline \beta\\\cline{1-1}\end{array}$	$\frac{1}{\sqrt{3}}$	0	0	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$D_{12}^{(0)*}$
$0,-1,-1$	$\begin{array}{\|c\|c\|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|}\hline \alpha&\gamma\\\hline \beta\\\cline{1-1}\end{array}$	$\frac{1}{\sqrt{3}}$	1	-1	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$D_{22}^{(0)*}$

If the phase of $\psi_1^{(0)-1}$ had not been chosen appropriately, say if it was chosen opposite to that given in Table 3.9, and if we still used (3-198) to obtain matrix elements from $u_{\nu mk,a}$, we would have obtained

$$D'(13) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \tag{3-220}$$

and $D'(13)D'(13)$ would be equal to $-I/2$ (I being the unit matrix) destroying the homomorphism $(13)(13) \to e$. Thus the last result is incorrect.

For the latter phase choice, we have to calculate the matrix elements from (3-188b). For example, we can obtain

$$D^{(0)1}(13) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, \quad D^{(0)-1}(13) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}. \tag{3-221a}$$

Now the irreps $D^{(0)1}$ and $D^{(0)-1}$ are no longer identical, but are only equivalent.

Ex. 3.10. Find the similarity transformation matrix between the irreps $D^{(0)1}$ and $D^{(0)-1}$.

Ex. 3.11. Prove the identities

$$\frac{1}{n}\sum_{k=0}^{n-1}(\rho_\mu^*\rho_m)^k = \delta_{m,\mu(\mathrm{mod}\ n)},\ \rho_m = \exp(-\tfrac{2m\pi i}{n}), \tag{3-221b}$$

$$\frac{1}{n}\sum_{k=0}^{n-1}\exp(-\tfrac{2m\pi i}{n}) = \delta_{m,0(\mathrm{mod}\ n)}. \tag{3-221c}$$

Hint: Applying the first orthogonality of irreducible matrices to the cyclic group C_n.

Ex. 3.12. From Table 3.9, write out all the irreducible matrices of S_3.

Ex. 3.13. Check Eqs. (3-214) and (3-215) for S_3.

Ex. 3.14. Find the $\mathcal{C}_{3v} \supset \mathcal{C}_3$ irreps by decomposing the regular rep of $\mathcal{C}_{3v}$ and compare the result with Ex. 3.4.

Ex. 3.15. For the quaternion group Q (1-4b) (a) Find two forms of the CSCO–III, one in the form of (3-166a) and the other in the form of (3-167a). (b) Decompose the regular rep of the matrix group Q. (c) Discuss the relation between the two–dimensional irreps of Q and the Pauli matrices.

Ex. 3.16. Repeat Ex. 3.15(a) and (b), but for the group $\mathcal{C}_{4v}$ (See Fig. 1.1-3). Also find the irreps for the following two subgroup chains: (1) $\mathcal{C}_{4v} \supset (e, \sigma_1)$; (2) $\mathcal{C}_{4v} \supset \mathcal{C}_4$ and compare the results with those of Ex. 3.5.

3.10. The Projection Operator $P^{(\nu)}_{mk}$ and the Generalized Projection Operator $\mathcal{P}^{(\nu)}_{m\kappa}$

3.10.1. Properties of the $P^{(\nu)}_{mk}$

Define the quantity

$$P^{(\nu)}_{mk} = \sqrt{\frac{h_\nu}{g}} P^{(\nu)k}_m = \frac{h_\nu}{g} \sum_a D^{(\nu)*}_{mk}(R_a) R_a \ . \tag{3-222}$$

From (3-196) one has

$$P^{(\nu)}_{mi} P^{(\mu)}_{jk} = \delta_{\nu\mu}\delta_{ij} P^{(\nu)}_{mk} \ . \tag{3-223}$$

Taking the hermitian conjugate of (3-222) and using the unitarity of R_a and $D^{(\nu)}$, we obtain

$$\begin{aligned} (P^{(\nu)}_{mk})^\dagger &= \frac{h_\nu}{g} \sum_a D^{(\nu)}_{mk}(R_a) R^\dagger_a = \frac{h_\nu}{g} \sum_a D^{(\nu)}_{mk}(R^{-1}_a) R_a \\ &= \frac{h_\nu}{g} \sum_a D^{(\nu)*}_{km}(R_a) R_a = P^{(\nu)}_{km} \ . \end{aligned} \tag{3-224}$$

There are many names for the operator $P^{(\nu)}_{mk}$, such as the normal unit operator (Rutherford 1948), unit operator (Dirl 1977), shift operator (Bohr 1969), or the irreducible symmetry operator (Melvin 1956). We prefer to call it the *projection operator.*

From (3-136) and (3-197) it is seen that, acting upon the intrinsic state $\Phi_0(X)$, $P^{(\nu)k}_m$ yields the $G \supset G(s)$ and $\overline{G} \supset \overline{G}(s)$ irreducible basis,

$$\psi^{(\nu)k}_m(X) = P^{(\nu)k}_m \Phi_0(X) \ . \tag{3-225}$$

It should be stressed that the meaning of the intrinsic quantum number k in configuration space depends on the choice of the intrinsic state. For example, applying $P^{(\nu)}_{mk}$ to another state $\varphi_a(X) = R_a \Phi_0(X)$, we obtain another state, namely,

$$\phi^{(\nu)k}_m(X) = P^{(\nu)k}_m \varphi_a(X) \ . \tag{3-226a}$$

This is still a $G \supset G(s)$ irreducible basis (ν, m), but is not a $\overline{G} \supset \overline{G}(s)$ irreducible basis (ν, k) with $\Phi_0(X)$ as the intrinsic state. From (3-225) and (3-197b), $\phi^{(\nu)k}_m$ can be expressed as a linear combination of the $\overline{G} \supset \overline{G}(s)$ irreducible basis $\psi^{(\nu)k}_m$ with $\Phi_0(X)$ as the intrinsic state,

$$\phi^{(\nu)k}_m(X) = \sum_{k'} D^{(\nu)}_{kk'}(\overline{R_a}) \psi^{(\nu)k'}_m(X) \ . \tag{3-226b}$$

Since the choice of the intrinsic state is arbitrary, we may choose $\varphi_a(X)$ as the intrinsic state $\Phi'_0(X)$. Thus $\phi^{(\nu)k}_m$ is the $\overline{G} \supset \overline{G}(s)$ irreducible basis (ν, k) with $\varphi_a(X)$ as the intrinsic state.

In Sec. 3.7.6 we introduced the I–, U–, and V–spin representations. From (3-226b) we can easily obtain the relations between the wave functions in different representations. Using

$$\Phi_0(U) = (132)\Phi_0(I), \quad \Phi_0(V) = (123)\Phi_0(I) ,$$

and letting $R_a = (132)$ and (123) in (3-226b), we have

$$\psi_m^{(\nu)k}(U) = \sum_{k'} D_{kk'}^{(\nu)}(132)\psi_m^{(\nu)k'}(I), \quad \psi_m^{(\nu)k}(V) = \sum_{k'} D_{kk'}^{(\nu)}(123)\psi_m^{(\nu)k'}(I) . \tag{3-226c}$$

The name of the shift operator for $P_{mk}^{(\nu)}$ comes from the following fact: By using (3-222), (3-223) and (3-225), we have

$$P_{lm'}^{(\nu)}\psi_m^{(\nu)k} = \sqrt{\frac{g}{h_\nu}} P_{lm'}^{(\nu)} P_{mk}^{(\nu)} \Phi_0 = \delta_{mm'}\psi_l^{(\nu)k} , \tag{3-227}$$

that is, when $m = m'$, the operator $P_{lm}^{(\nu)}$ shifts the m–th component to the l–the component of the (ν) irreducible basis.

From (3-200b) we obtain the inverse of (3-222):

$$R_a = \sum_{\nu=1}^{N} \sum_{m,k=1}^{h_\nu} D_{mk}^{(\nu)}(R_a) P_{mk}^{(\nu)} . \tag{3-228}$$

Letting $R_a = e$, we deduce the decomposition of the identity element, i.e.,

$$e = \sum_{\nu=1}^{N} \sum_{m=1}^{h_\nu} P_{mm}^{(\nu)} . \tag{3-229}$$

From (3-224) and (3-223), we find

$$(P_{mm}^{(\nu)})^\dagger = P_{mm}^{(\nu)} , \tag{3-230}$$

$$P_{mm}^{(\nu)} P_{ll}^{(\nu)} = \delta_{ml} P_{mm}^{(\nu)} . \tag{3-231}$$

This shows that $P_{mm}^{(\nu)}$ is a self-adjoint idempotent, called the *primitive idempotent*. $P_{mm}^{(\nu)}$ is a projection operator onto the m–th component of the m–th ν irreducible basis, $\psi_m^{(\nu)m} = P_{mm}^{(\nu)}\Phi_0$. It should be emphasized that neither $\{P_{mm}^{(\nu)} : m = 1, 2, \ldots, h_\nu\}$ nor $\{P_{mm}^{(\nu)}\Phi(X) : m = 1, 2, \ldots, h_\nu\}$ with arbitrary $\Phi(X)$ forms an irreducible basis. Only when the irrep (ν) occurs once in the rep space $\{R_a\Phi(X) : a = 1, 2, \ldots, g\}$ does $\{P_{mm}^{(\nu)}\Phi(X) : m = 1, 2, \ldots, h_\nu\}$ form an irreducible basis.

From (3-197a), it follows that

$$R_a P_{kk}^{(\nu)} = \sum_{k'} D_{k'k}^{(\nu)}(R_a) P_{k'k}^{(\nu)} . \tag{3-232}$$

Thus the set $\{R_a P_{kk}^{(\nu)} : a = 1, 2, \ldots, g\}$ belongs to the k–th ν–irreducible space $L_{(\nu)k}$, and $P_{kk}^{(\nu)}$ is the generator of the subspace $L_{(\nu)k}$. Equation (3-229) corresponds to the decomposition of L_g into a direct sum of the irreducible spaces of $G, L_g = \sum_{\nu k} \oplus L_{(\nu)k}$. In a parallel way, $\{P_{mm}^{(\nu)} R_a : a = 1, 2, \ldots, g\}$ belongs to the irreducible space $\overline{L}_{(\nu)m}$ of the intrinsic group $\overline{G}$, and Eq. (3-229) also corresponds to the decomposition of L_g into a direct sum of the irreps of $\overline{G}, L_g = \Sigma_{m\nu} \oplus \overline{L}_{(\nu)m}$.

Let us define

$$P^{(\nu)} = \sum_{k=1}^{h_\nu} P_{kk}^{(\nu)} . \tag{3-233}$$

From (3-231) it is readily seen that

$$P^{(\nu)}P^{(\mu)} = \delta_{\nu\mu}P^{(\nu)} \ . \tag{3-234}$$

The idempotent $P^{(\nu)}$ is the generator of the eigenspace L_ν of the CSCO of G, and (3-233) corresponds to the decomposition (3-174).

From Eqs. (2-90), (3-222) and the definition of $P^{(\nu)}$ in (3-233),

$$P^{(\nu)} = \frac{h_\nu}{g}\sum_{i=1}^{N}\chi_i^{(\nu)*}C_i \ . \tag{3-235a}$$

Obviously, $P^{(\nu)}$ is the eigenoperator of the CSCO of G with the eigenvalue ν and (3-234) is precisely (3-52). Therefore, the operator $P^{(\nu)}$ in (3-233) which is obtained from a contraction of $P_{kk}^{(\nu)}$ is identical to $P^{(\nu)} = Q^{(\nu)}/\eta_\nu$ in (3-51). $P^{(\nu)}$ is also called *projection operator.*

Comparing the last result with Eqs. (3-51) and (3-27b), one has

$$\frac{h_\nu}{g}\chi_i^{(\nu)*} = \frac{1}{\eta_\nu}q_i^{(\nu)} \ . \tag{3-236}$$

Setting $m = k$ and $m' = k'$ in (3-200a) and summing over m and m', one gets

$$\sum_{i=1}^{N}\frac{g_i}{g}\chi_i^{(\nu)*}\chi_i^{(\nu')} = \delta_{\nu\nu'} \ . \tag{3-237a}$$

Hence we see that if $(g_i/g)^{\frac{1}{2}}\chi_i^{(\nu)}(i,\nu = 1,2,\ldots,N)$ are regarded as matrix elements of a $N \times N$ matrix, then any two row vectors of the matrix are orthonormal. According to a general theorem of linear algebra, any two column vectors of such a matrix are necessarily also orthonormal, that is,

$$\sum_{\nu=1}^{N}\frac{g_i}{g}\chi_i^{(\nu)*}\chi_j^{(\nu)} = \delta_{ij} \ . \tag{3-237b}$$

Equations (3-237a,b) are the two *orthogonality theorems* for characters. Either may be used as a criterion for the irreducibility of a rep.

Using (3-237b) we are able to find the inverse of Eq. (3-235a):

$$C_i = \sum_{\nu=1}^{N}\frac{g_i}{h_\nu}\chi_i^{(\nu)}P^{(\nu)} \ . \tag{3-235b}$$

Since the characters of the inequivalent irreps form an orthogonal vector system, two inequivalent irreps cannot have the same characters and irreps with equal characters are equivalent. From Sec. 2.8 we also know that equivalent reps have equal characters. Therefore we have

Theorem 3.28: The equality of the characters is a necessary and sufficient condition for two irreps to be equivalent.

In addition, (3-69) shows that the simple characters are uniquely decided by the eigenvalues of the CSCO of G. Consequently we have

Theorem 3.29: The equality of the eigenvalue ν of the CSCO of G is the necessary and sufficient condition for two irreps to be equivalent.

3.10.2. A recursive method for constructing the $P_{mk}^{(\nu)}$

When the simple characters of a group G are known and those of its subgroups contained in a canonical subgroup chain $G(s)$ are also known, the following recursive method (Chen 1979)

can be used for constructing the projection operator $P^{(\nu)}_{mk}$ without solving the eigenequations (3-169a).

Suppose the canonical subgroup chain can be written $G(s) = G(1) \supset G(2) \supset, \ldots$, with the CSCO $C(s) = \big(C(1), C(2)\ldots\big)$. Their irreps are labeled by $(\nu_1, \nu_2, \ldots)$. Then up to a constant factor we have

$$\begin{aligned} P^{(\nu)}_{mm} &= P^{(\nu)} P^{(\nu_1)} P^{(\nu_2)} \ldots , \\ m &= (\nu_1, \nu_2, \nu_3, \ldots) . \end{aligned} \tag{3-238}$$

Proof: From $[C, C(i)] = 0, [C(i), C(j)] = 0, i, j = 1, 2, \ldots$ and Eq. (3-235a), we know that $C(i)$ commutes with any factor $P^{(\nu_j)}$ in (3-238). Therefore

$$\begin{aligned} & C P^{(\nu)}_{mm} = \nu P^{(\nu)}_{mm}, \\ & C(i) P^{(\nu)}_{mm} = P^{(\nu)} P^{(\nu_1)} \ldots (C(i) P^{(\nu_i)}) \ldots = \nu_i P^{(\nu)}_{mm} , \\ & \overline{C}(i) P^{(\nu)}_{mm} = P^{(\nu)}_{mm} C(i) = \nu_i P^{(\nu)}_{mm} , \end{aligned} \tag{3-239}$$

which is a special case of (3-169a).

Let $P^{(\nu_1)}_{m_1 m_1}$ be the projection operator of G_1 for the subgroup chain $G(1) \supset G(2) \supset G(3) \supset, \ldots$, then we have

$$P^{(m)} \equiv P^{(\nu_1)}_{m_1 m_1} = P^{(\nu_1)} P^{(\nu_2)} P^{(\nu_3)} \ldots , \tag{3-240a}$$

where $m = (\nu_1, \nu_2, \nu_3, \ldots)$, $m_1 = (\nu_2, \nu_3, \ldots)$. From (3-238) and (3-240a) we have

$$P^{(\nu)}_{mm} = P^{(\nu)} P^{(m)} = P^{(\nu)} P^{(\nu_1)}_{m_1 m_1} . \tag{3-240b}$$

This shows that the idempotent $P^{(\nu)}_{mm}$ of G is expressible in terms of the projection operator of G and the idempotent $P^{(\nu)}_{m_1 m_1}$ of its subgroup $G(1)$. Thus a recursive procedure is established. **QED**

Similarly, up to a constant factor we have

$$\begin{aligned} P^{(\nu)}_{mk} &= P^{(\nu)} P^{(m)} R P^{(k)} , \\ P^{(k)} = P^{(\bar{\nu}_1)} P^{(\bar{\nu}_2)} P^{(\bar{\nu}_3)} \ldots , \quad & k = (\bar{\nu}_1, \bar{\nu}_2, \bar{\nu}_3, \ldots) , \end{aligned} \tag{3-241}$$

where R is an appropriate element of G and can be chosen freely so long as $P^{(m)} R P^{(k)} \neq 0$.

Example: The group S_3. Ignoring the constant factors, from Eq. (3-44a) we have the projection operators of S_3 and S_2,

$$\begin{aligned} P^{(\nu)} = P^{(0)} &= (2e - (123) - (132)) . \\ P^{(m)} = P^{(\pm 1)} &= (e \pm (12)). \end{aligned}$$

Therefore

$$\begin{aligned} P^{(0)}_{1,1} = P^{(0)} P^{(1)} &= [2(e + (12)) - (13) - (23) - (123) - (132)] . \\ P^{(0)}_{-1,1} &= P^{(0)} P^{(-1)} (23) P^{(1)} \\ &= [2e - (123) - (132)][e - (12)](23)[e + (12)] \\ &= 3[-(13) + (23) - (123) + (132)] , \end{aligned}$$

in agreement with Table 3.9.

This method is used extensively in the book by Harter (1993 Sec. 3.3) for point groups. An disadvantage of this method is that it is quite tedious for hand calculation and is rather hard to have it coded.

Ex. 3.17. Using the result of Ex. 3.1, find the primitive idempotents $P^{(2)}_{mm}$ of S_4 for $m = (3,1), (0,1)$ and $(0,-1)$.

3.10.3. Generalized irreducible matrices and generalized projection operator

The operator

$$\mathcal{P}^{(\nu)}_{m\kappa} = \frac{h_\nu}{g} \sum_a \mathcal{D}^{(\nu)*}_{m\kappa}(R_a) R_a \tag{3-242a}$$

is called the *generalized projection operator*, where $\mathcal{D}^{(\nu)*}_{m\kappa}(R_a)$ is the matrix elements of a group operator R_a between two irreducible basis vectors adapted to *different subgroup chains*,

$$\mathcal{D}^{(\nu)}_{m\kappa}(R_a) = \langle \psi^{(\nu)}_m | R_a | \phi^{(\nu)}_\kappa \rangle \ , \tag{3-242b}$$

where $\psi^{(\nu)}_m$ and $\varphi^{(\nu)}_\kappa$ are the $G \supset G(s)$ and $G \supset G(s)'$ irreducible bases, respectively. The $\mathcal{D}^{(\nu)}_{m\kappa}(R_a)$ are called the *generalized* (or *skew*) *irreducible matrix elements* (Klein 1982) . In analogy with Eq. (3-205), it can be shown that $\mathcal{D}^{(\nu)}_{m\kappa}(R_a)^*$ satisfies the following eigenequations

$$\begin{pmatrix} C \\ C(s) \\ \overline{C}(s)' \end{pmatrix} \mathcal{D}^{(\nu)}_{m\kappa}(R_a)^* = \begin{pmatrix} \nu \\ m \\ \kappa \end{pmatrix} \mathcal{D}^{(\nu)}_{m\kappa}(R_a)^* \ , \tag{3-242c}$$

where $C(s)'$ is the CSCO of the subgroup chain $G(s)'$.

From (3-242c) and a normalization condition similar to (3-200a) with D replaced by $\mathcal{D}$, we can evaluate the generalized matrix elements.

Similar to (3-223) and (3-224) we have

$$\mathcal{P}^{(\nu)}_{m\kappa}\mathcal{P}^{(\mu)}_{\kappa' m'} = \delta_{\nu\mu}\delta_{\kappa\kappa'} P^{(\nu)}_{mm'} \quad (\mathcal{P}^{(\nu)}_{m\kappa})^\dagger = \mathcal{P}^{(\nu)}_{\kappa m} \ , \tag{3-242d}$$

which transform a $G \supset G(s)'$ basis vector $\phi^{(\nu)}_\kappa$ to the $G \supset G(s)$ basis vector $\psi^{(\nu)}_m$,

$$\psi^{(\nu)}_m = \text{const} \times \delta_{\kappa\kappa'} \mathcal{P}^{(\nu)}_{m\kappa} \phi^{(\nu)}_{\kappa'} \ . \tag{3-242e}$$

Both the projection operator $P^{(\nu)}_{mm'}$ and the generalized projection operator $\mathcal{P}^{(\nu)}_{m\kappa}$ can be used to project out the $G \supset G(s)$ irreducible basis from a reducible basis vector φ_0,

$$\psi^{(\nu)}_m = \text{const} \times P^{(\nu)}_{mm'} \varphi_0 = \text{const} \times \mathcal{P}^{(\nu)}_{m\kappa} \varphi_0 \ . \tag{3-242f}$$

Since the multiplicity separation can be chosen freely, it gives us a flexibility in choosing the intrinsic subgroup chain $\bar{G} \supset \bar{G}(s)$ so that the projection operator becomes as simple as possible. For example, if one needs to find irreducible basis for a non-canonical group chain $G \supset G(s)'$, it will be convenient to use the $G \supset G(s)'$ and $\bar{G} \supset \bar{G}(s)$ projection operator $\mathcal{P}^{(\nu)}_{\kappa m}$ instead of $P^{(\nu)}_{\kappa\kappa'}$, where $G \supset G(s)$ is assumed to be canonical. In Sec. 4.18.3 and Sec. 8.5 we will see that the generalized projection operator is very useful.

3.10.4. Coset factored projection operator

Suppose we have a group chain $G \supset H \supset K$ with the quantum numbers ν, Λ and ρ for the groups G, H and K, respectively, and K is an Abelian group. The $G \supset H \supset K$ projection operator $\mathbf{P}^{(\nu)}_{\Lambda\rho,\bar{\Lambda}\bar{\rho}}$ involves a summation over all the $|G|$ elements and is rather cumbersome. Using the coset decomposition, the expression for the projection operator $G \supset H \supset K$ can be greatly simplified.

Using the left-coset decomposition $G = (e + s_2 + s_3 + \cdots)H$ [see (1-24)], we can get the

left-coset factored projection operator:

$$\begin{aligned}\mathbf{P}^{(\nu)}_{\Lambda\rho,\bar{\Lambda}\bar{\rho}} &= \frac{h_\nu}{|G|}\sum_{a=1}^{|G|} D^{(\nu)}_{\Lambda\rho,\bar{\Lambda}\bar{\rho}}(R_a)^* R_a \\ &= \frac{h_\nu}{|G|}\sum_{h\in H}\sum_{i,\rho'} D^{(\nu)}_{\Lambda\rho,\bar{\Lambda}\rho'}(s_i)^* D^{(\nu)}_{\bar{\Lambda}\rho',\bar{\Lambda}\bar{\rho}}(h)^* s_i h \\ &= \frac{|H|}{|G|}\frac{h_\nu}{h_\Lambda}\sum_{i,\rho'} D^{(\nu)}_{\Lambda\rho,\bar{\Lambda}\rho'}(s_i)^* s_i P^{(\bar{\Lambda})}_{\rho'\bar{\rho}} ,\end{aligned} \tag{3-243a}$$

where we used $D^{(\nu)}_{\bar{\Lambda}'\rho',\bar{\Lambda}\bar{\rho}}(h) = \delta_{\bar{\Lambda}\bar{\Lambda}'} D^{(\bar{\Lambda})}_{\rho'\bar{\rho}}(h)$. Similarly we have the right-coset factored projection operator

$$\mathbf{P}^{(\nu)}_{\Lambda\rho,\bar{\Lambda}\bar{\rho}} = \frac{|H|}{|G|}\frac{h_\nu}{h_\Lambda}\sum_{i,\rho'} D^{(\nu)}_{\Lambda\rho',\bar{\Lambda}\bar{\rho}}(s_i)^* P^{(\Lambda)}_{\rho\rho'} s_i, \tag{3-243b}$$

The projection operator can also be cast into double-coset factored form, see (8-59).

3.11. The Eigenfunction Method for Characters

The EFM given in this section provides a simple method for computing characters of finite groups. From (3-236), (3-54), and (3-67), one has

$$|\eta_\nu|^2 = \frac{g}{h_\nu^2} . \tag{3-244a}$$

Choosing η_ν to be real and positive, we find

$$\eta_\nu = \sqrt{g}/h_\nu . \tag{3-244b}$$

Substituting this into (3-236), one obtains the relation between the simple character $\chi_i^{(\nu)}$ and the eigenvector $q_i^{(\nu)}$,

$$\chi_i^{(\nu)} = \sqrt{g} q_i^{(\nu)*} . \tag{3-245}$$

Thus the problem of finding characters is converted into that of finding the eigenvectors of the CSCO of G in class space.

If the simple characters $\chi_i^{(\nu)}$ are regarded as a function $\chi^{(\nu)}(C_i)$ on the classes, then from (3-205) we know that the complex conjugate of the simple character is an eigenfunction of the CSCO of G,

$$C\chi^{(\nu)*}(C_i) = \nu\chi^{(\nu)*}(C_i) . \tag{3-246}$$

Equation (3-246) remains true for compact Lie groups.

The EFM for characters is as follows:

1. Find the representatives of the l class operators in the CSCO of $G, C = (C_{i_1}, C_{i_2}, \ldots, C_{i_l})$,

$$\| C^k_{i_1,j} \|_1^N, \ \| C^k_{i_2,j} \|_1^N, \ldots .$$

2. Find the simultaneous eigenvectors using

$$\sum_j (C^k_{ij} - \lambda_i^{(\nu)}\delta_{jk}) q_j^{(\nu)} = 0, \quad i = i_1, i_2, \ldots . \tag{3-247}$$

Choose them so they have normalization $\sum_{i=1}^N g_i |q_i^{(\nu)}|^2 = 1$ and make the phase choice such that $q_e^{(\nu)}$ is real and positive.

3. From $\chi_i^{(\nu)} = \sqrt{g} q_i^{(\nu)*}$, we obtain the characters.

For example, according to (3-245), from (3-44a), (3-46) and (3-49) we can easily obtain the simple characters of $S_3 (g = 6)$ and $\mathcal{C}_{6v} (g = 12)$, listed in Tables 3.11-1 and 3.11-2.

Table 3.11-1. Character table of S_3.

$\lambda^{(\nu)}$	class / partitions	C_1 (1^3)	C_2 (12)	C_3 (3)
3	[3]	1	1	1
−3	$[1^3]$	1	−1	1
0	[21]	2	0	−1

Table 3.11-2. Character table of $\mathcal{C}_{6v}$.

$\lambda_4^{(\nu)}$	$\lambda_5^{(\nu)}$	class / old labels	C_1	C_2	C_3	C_4	C_5	C_6
2	3	A_1	1	1	1	1	1	1
2	−3	A_2	1	1	1	1	−1	−1
−2	3	B_1	1	−1	1	−1	1	−1
−2	−3	B_2	1	−1	1	−1	−1	1
−1	0	E_1	2	2	−1	−1	0	0
1	0	E_2	2	−2	−1	1	0	0

Before the EFM was proposed, several conventional methods were available for determining the simple characters. These included (a) Jones' method (1975), (b) Boerner's method (1963), (c) Bradley and Cracknell's method (1972), (d) Burnside's method (1955) and (e) Dixon's method (1967). The EFM differs from these methods in the introduction of the CSCO for the class space, which greatly simplifies the calculation.

Ex. 3.18. Find the simple characters of S_4 (using the results of Ex. 3.1).

Ex. 3.19. Find the simple characters of $\mathcal{C}_{4v}$.

3.12. Applications of Simple Characters

From the previous discussion, we see that in the new approach to group representation theory, the concept of character does not play the dominant role it has in traditional group theory. We can carry out the reduction of a rep of G without any knowledge of the simple characters. However, if the simple characters are known, as is the case with all commonly used finite groups, then they can be used to simplify calculations.

The simple characters have the following major applications in the new approach.

1. Finding the CSCO of G. From the character table and the relation $\lambda_i^{(\nu)} = (g_i/h_\nu)\chi_i^{(\nu)}$, we can construct the following matrix,

$$\begin{pmatrix} \lambda_1^{(\nu_1)} & \lambda_2^{(\nu_1)} & \cdots & \lambda_N^{(\nu_1)} \\ \lambda_1^{(\nu_2)} & \lambda_2^{(\nu_2)} & \cdots & \lambda_N^{(\nu_2)} \\ \cdots & \cdots & \cdots & \cdots \\ \lambda_1^{(\nu_N)} & \lambda_2^{(\nu_N)} & \cdots & \lambda_N^{(\nu_N)} \end{pmatrix} . \tag{3-248}$$

If we can find a column in the matrix, say column i_1, which has N distinct eigenvalues, then the class operator C_{i_1} is a CSCO of G. Otherwise, we look for two columns, say columns i_1 and i_2. If the N pairs of eigenvalues $(\lambda_{i_1}^{(\nu_1)}, \lambda_{i_2}^{(\nu_1)}), \ldots, (\lambda_{i_1}^{(\nu_N)}, \lambda_{i_2}^{(\nu_N)})$ are all different, then (C_{i_1}, C_{i_2}) is a CSCO of G, etc. Therefore, if the simple characters are known, it is trivial to find the CSCO of G.

2. Determining the multiplicity of an irrep in a reducible rep. In Eqs. (2-103b,c) we introduced the multiplicity τ_ν as the number of times the irrep (ν) occurs in a rep D with the characters χ_i,

$$D = \sum_\nu \oplus \tau_\nu D^{(\nu)} , \quad \chi_i = \sum_\nu \tau_\nu \chi_i^{(\nu)} . \tag{3-249a}$$

From (3-237) and (3-249a) we obtain an important expression for the multiplicity τ_ν,

$$\tau_\nu = \sum_i \frac{g_i}{g} \chi_i \chi_i^{(\nu)*} = \frac{1}{g} \sum_R \chi(R) \chi^{(\nu)}(R)^* . \tag{3-249b}$$

If we are only interested in which irreps a given rep will decompose into, we can get the answer from our last result without solving the eigenfunction of the CSCO of G.

Example: Find the multiplicity τ_ν of the irrep (ν) in the regular rep of G.

The answer is already known to be $\tau_\nu = h_\nu$. Here we merely use (3-249b) to check the result. From Sec. 2.6.1 we know that in the regular rep only the identity has a non-vanishing character,

$$\chi_e = g ; \quad \chi_i = 0 , \quad i \neq e .$$

Using $g_e = 1$ and $\chi_e^{(\nu)} = h_\nu$, from (3-249b) we get $\tau_\nu = h_\nu$.

Equation (3-249b) tells us that if two reps have equal characters, then both will have the same block-diagonal form (2-101) after reduction, and therefore are identical except for the order of appearance of $D^{(\nu_i)}(R)$. Thus they can be transformed into an equivalent reduced form and, therefore, are themselves equivalent. On the other hand, two equivalent reps must have the same characters. Thus we have the generalization of Theorem 3.28.

Theorem 3.30: The equality of characters is a necessary and sufficient condition for the equivalence of two reps.

Irreps are divided into three *types* according to three possible relations between an irrep and its complex conjugate (Loewy 1903, Wigner 1932, Wigner 1959). An irrep ν is said to be

a. *Potential real or self-conjugate real*: If (ν) is equivalent to its complex conjugate rep $(\nu)^*$ and to a real rep as well.

b. *Pseudo real or self-conjugate complex*: If (ν) is equivalent to its complex conjugate rep $(\nu)^*$ but not to any real rep.

c. *complex, or non self-conjugate*: If the irrep (ν) and $(\nu)*$ are inequivalent.

An irrep with complex character is necessarily not equivalent to its complex conjugate with the characters $\chi^{(\nu)*}$ (since $\chi^{(\nu)} \neq \chi^{(\nu)*}$) and thus belong to the type *c*.

The criterion for the types of irreps was first discovered by Loewy (1903) and discussed in many publications (Wigner 1959, Hamermesh 1962, Bradley 1972):

Theorem 3.31:

$$\frac{1}{|G|} \sum_{a=1}^{|G|} \chi^{(\nu)}(R_a^2) = \begin{cases} 1 & \text{if and only if } (\nu) \text{ is of type } a. \\ -1 & \text{if and only if } (\nu) \text{ is of type } b. \\ 0 & \text{if and only if } (\nu) \text{ is of type } c. \end{cases} \tag{3-250}$$

The types of all irreps of point groups are listed in Table 8.3-1 to Table 8.3-9. The importance of classifying irreps into types will be discussed in Sec. 8.13 in connection with the time reversal symmetry.

3.13. Reduction of Non-Regular Reps (The EFM for Irreducible Bases)

3.13.1. Multiplicity free case ($\tau_\nu = 1$)

Suppose that there are n orthonormal wave functions,

$$\varphi_a(X) , \quad a = 1, 2, \ldots n , \tag{3-251a}$$

which carry a reducible rep of G and the irrep ν occurs only once in the reducible rep, and that we need to find the irreducible basis

$$\psi_m^{(\nu)} = \sum_a u_{\nu m,a}\varphi_a \ , \tag{3-251b}$$

adapted to a canonical subgroup chain $G \supset G(s)$. The basis functions $\psi_m^{(\nu)}$ satisfy

$$\begin{pmatrix} C \\ C(s) \end{pmatrix} \psi_m^{(\nu)} = \begin{pmatrix} \nu \\ m \end{pmatrix} \psi_m^{(\nu)} \ , \tag{3-252a}$$

or

$$\sum_{b=1}^{N} \left[\left\langle \varphi_a \left| \begin{matrix} C \\ C(s) \end{matrix} \right| \varphi_b \right\rangle - \begin{pmatrix} \nu \\ m \end{pmatrix} \delta_{ab} \right] u_{\nu m,b} = 0 \ . \tag{3-252b}$$

If the eigenvalue (ν, m) is a single root, it means that the irrep ν occurs only once, and the h_ν eigenvectors $\psi_m^{(\nu)}$ carry the irrep ν of G.

A distinguishing feature of the EFM is that for obtaining irreducible basis we do not need any knowledge of the irreducible matrices. For example, with the EFM the $S_6 \supset O_h \supset C_4$ irreducible basis has been obtained in Ping & Chen 1997, where O_h is the octahedral group (Sec. 8.2), in spite of the fact that irreducible matrices of the permutation group S_6 in the "exotic" group chain $S_6 \supset O_h \supset C_4$ are unknown.

In the foregoing procedure, a knowledge of the irreducible matrices is not necessary. However, in some cases, certain conventional or standard irreducible matrices for the $G \supset G(s)$ basis are given. We can use the following technique to ensure that the irreducible basis found from the EFM is consistent (including the phase) with the standard matrices.

We need only find one component from (3-252), say $\psi_m^{(\nu)}$. Using the known matrix elements, we can construct an operator $F_{m'm}(R)$ as a suitable linear combination of the group elements. The operator $F_{m'm}(R)$ can be used to derive the other components successively from the known component m,

$$\psi_{m'}^{(\nu)} = F_{m'm}^{(\nu)}(R)\psi_m^{(\nu)} \ . \tag{3-253a}$$

The form of the operator $F_{m'm}^{(\nu)}(R)$ is very simple for the common finite groups, and can be easily found. For example, suppose that $R_a\psi_m^{(\nu)} = c_1\psi_m^{(\nu)} + c_2\psi_{m'}^{(\nu)}$; then

$$F_{mm'}^{(\nu)}(R) = (R_a - c_1)/c_2 \ . \tag{3-253b}$$

3.13.2. Canonical subgroup chains with $\tau_\nu > 1$

Suppose that the eigenvalue (ν, m) is a τ_ν-fold root; then this fact indicates that the irrep ν occurs τ_ν times, and for a given (ν, m), there are τ_ν linearly independent solutions to (3-252),

$$\psi_m^{(\nu)\tau} \ , \quad \tau = 1, 2, \ldots, \tau_\nu \ .$$

The eigenvectors $\psi_m^{(\nu)\tau}$ can be chosen to be orthogonal in the multiplicity label τ. However, it should be stressed that the eigenvectors $\psi_m^{(\nu)\tau}, m = 1, 2, \ldots, h_\nu$, chosen arbitrarily except for the requirement of orthogonality with respect to τ, in general do not generate an irrep of G. To obtain the irreducible basis we can use either of the following two methods.

Method One. Using intrinsic quantum numbers: In reducing a regular rep, the h_ν distinct eigenvalues k of $C(s)$ provide just enough labels for distinguishing the h_ν equivalent irreps. In reducing a non-regular rep, an irrep ν may occur only $\tau_\nu < h_\nu$ times. For such cases, there are too many intrinsic quantum numbers k. Now the question is; Can we still use the intrinsic quantum number to distinguish the τ_ν equivalent irreps? If the answer is yes, then how?

For non-regular reps, the intrinsic state $\Phi_0(X)$ must have certain symmetries (otherwise applying $|G|$ elements to it will generate $|G|$ basis vectors carrying the regular rep of G). Suppose that it is invariant under a set of elements $\{T_\alpha : \alpha = 1, 2, \ldots |G_{in}|\}$,

$$T_\alpha \Phi_0(X) = \Phi_0(X), \quad T_\alpha \in G_{in} \ . \tag{3-254}$$

The set forms a subgroup G_{in} of the group G, called the *symmetry group of the intrinsic state.* The left coset decomposition of G with respect to G_{in} is denoted as

$$G = \sum_{i=1}^{q} \oplus a_i G_{in} \ , \quad a_1 = e \ . \tag{3-255a}$$

Applying the $|G|$ elements R to $\Phi_0(X)$ we can get only $q = |G|/|G_{in}|$ linearly independent states φ_i which carry a non-regular rep of G,

$$\varphi_i = a_i \Phi_0(X) \ . \tag{3-255b}$$

Let us now inspect the action of an intrinsic group element $\overline{R}$ on the basis vector $\varphi_1 = \Phi_0(X)$:

$$\begin{aligned} \overline{R}\Phi_0(X) &= R\Phi_0(X) \ . \\ \overline{R}\Phi_0(X) &= \overline{R}T_\alpha \Phi_0(X) = T_\alpha R \Phi_0(X) \ . \end{aligned} \tag{3-256}$$

Since in general $R\Phi_0(X) \neq T_\alpha R \Phi_0(X)$, unless R belongs to the symmetry group G_{in}, a contradiction arises here. Therefore, the intrinsic group elements do not have a definite meaning in the non-regular rep space, except those which belong to the intrinsic subgroup G_{in} and thus are equivalent to the identity.

For example, the symmetry group for the intrinsic state $\Phi_0 = |\alpha\beta\beta\gamma\rangle$ is $G_{in} = \{e, (23)\}$. The intrinsic permutation $(\overline{12})$ is meaningless,

$$\begin{aligned} (\overline{12})\Phi_0 &= (12)\Phi_0 = (12)|\alpha\beta\beta\gamma\rangle = |\beta\alpha\beta\gamma\rangle \ , \\ (\overline{12})\Phi_0 &= (\overline{12})(23)\Phi_0 = (23)(12)\Phi_0 = |\beta\beta\alpha\gamma\rangle \ . \end{aligned}$$

Nevertheless, according to the following theorem, we can still extract out of the intrinsic group something which remains meaningful in the non-regular rep space.

Theorem 3.32: If the class operators $C_i(1)$ of a subgroup G_1 of G commute with the symmetry group G_{in} of the intrinsic state,

$$[C_i(1), T_\alpha] = 0 \ , \quad \alpha = 1, 2, \ldots, |G_{in}| \ , \tag{3-257}$$

then the class operators $\overline{C}_i(1)$ of the corresponding intrinsic group $\overline{G}_1$ have a consistent, and therefore definite, meaning.

Proof: According to Eq. (3-257) we have

$$\overline{C}_i(1)\Phi_a(X) = \overline{C}_i(1)R_a\Phi_0(X) = R_a C_i(1)\Phi_0(X) \ . \tag{3-258}$$

$$\begin{aligned} \overline{C}_i(1)\Phi_a(X) &= \overline{C}_i(1)R_a T_\alpha \Phi_0(X) = R_a T_\alpha C_i(1)\Phi_0(X) \ . \\ &= R_a C_i(1) T_\alpha \Phi_0(X) = R_a C_i(1)\Phi_0(X) \ . \quad \textbf{QED} \end{aligned} \tag{3-259}$$

In summary, for the non-regular rep case, a meaningful operator set $\overline{C}(s')$ can be found using the following steps:

(a) Find the symmetry group G_{in} for the chosen intrinsic state $\Phi_0(X)$.

(b) Find the subgroup chain $G(s')$ whose CSCO, $C(s')$, commutes with G_{in}.

Stated differently, $G(s')$ results from deleting all those subgroups in the canonical subgroup chain $G(s)$ whose CSCO, denoted by $C(s'')$, do not commute with G_{in}.

(c) Then the corresponding intrinsic operator set $\overline{C}(s')$ has a definite meaning.

Obviously, $G \supset G(s')$ is no longer a canonical subgroup chain. For example, for the intrinsic state $|\alpha\beta\beta\gamma\rangle, G_{in} = \{e,(23)\}, G(s') = S_3$, and the meaningful operator set is $\overline{C}(s') = \overline{C}(3)$, in contrast to the regular rep case, for which $G(s) = S_3 \supset S_2$, and $\overline{C}(s) = (\overline{C}(3), \overline{C}(2))$.

In the case when single group elements have no definite meaning in a given space, we can no longer talk about irreducible bases of the group in the space. However, since the CSCO's of the intrinsic group $\overline{G}$ and the subgroup chain $\overline{G}(s')$ do have a definite meaning, for convenience in exposition, we call the simultaneous eigenfunction of $(\overline{C}, \overline{C}(s'))$ a $\overline{G} \supset \overline{G}(s')$ *quasi irreducible basis* .

Having found the meaningful operator set $\overline{C}(s')$, we can use it to lift the degeneracy of (ν, m) in Eq. (3-252).

Theorem 3.33: The set of operators $(C, C(s), \overline{C}(s'))$ is a CSCO for the non–regular rep space $\{a_i \Phi_0(X) : \ i = 1, 2 \ldots, q\}$.

Although we cannot yet prove this theorem, no counter examples have been found.

Therefore, the intrinsic operator set $\overline{C}(s')$ provides just enough quantum numbers for distinguishing the τ_ν equivalent irreps.

Equation (3-252) is extended to

$$
\begin{gathered}
\psi_m^{(\nu)\kappa} = \sum_a u_{\nu m\kappa,a} \varphi_a \ , \\
\begin{pmatrix} C \\ C(s) \\ \overline{C}(s') \end{pmatrix} \psi_m^{(\nu)\kappa} = \begin{pmatrix} \nu \\ m \\ \kappa \end{pmatrix} \psi_m^{(\nu)\kappa} \ . \\
\sum_{b=1}^{N} \left[\left\langle \varphi_a \left| \begin{matrix} C \\ C(s) \\ \overline{C}(s') \end{matrix} \right| \varphi_b \right\rangle - \begin{pmatrix} \nu \\ m \\ \kappa \end{pmatrix} \delta_{ab} \right] u_{\nu m\kappa,b} = 0 \ , \\
m = m_1, m_2, \ldots, m_{h_\nu}, \quad \kappa = \kappa_1, \kappa_2, \ldots, \kappa_{\tau_\nu} \ , \quad N = \sum_\nu \tau_\nu h_\nu \ .
\end{gathered}
\tag{3-260}
$$

Note the relation between the quantum number sets κ and k: κ results from deleting all the quantum numbers of the now meaningless operators $C(s'')$ in the set k.

The set of eigenvectors $\{\psi_m^{(\nu)\kappa} : \ m = 1, 2, \ldots, h_\nu\}$ is the $G \supset G(s)$ basis for the κ–th irrep ν. If the phases of the eigenvectors with different κ are chosen arbitrarily, the τ_ν irreps carried by the τ_ν sets of eigenvectors are only equivalent instead of being identical. For obtaining τ_ν sets of the $G \supset G(s)$ irreducible bases which will transform according to the same irrep $D^{(\nu)}$,

$$
R\psi_m^{(\nu)\kappa} = \sum_{m'} D^{(\nu)}_{m'm}(R) \psi_{m'}^{(\nu)\kappa} \ , \tag{3-261}
$$

we can use the technique introduced in the previous subsection. That is we only need to find the τ_ν eigenvectors $\psi_m^{(\nu)\kappa}, \kappa = 1, 2, \ldots, \tau_\nu$, for a particular component m and the other components can be obtained by recursively using the formula

$$
\psi_{m'}^{(\nu)\kappa} = F^{(\nu)}_{m'm}(R) \psi_m^{(\nu)\kappa} \ . \tag{3-262}
$$

Although (3-261) parallels (3-215), there is no counterpart of (3-214), since single intrinsic group elements have no meaning.

The q basis vectors $\psi_m^{(\nu)\kappa}$ form an orthonormal complete set in the non–regular rep space. The orthonormality relation is

$$
\langle \psi_{m'}^{(\nu')\kappa'} | \psi_m^{(\nu)\kappa} \rangle = \delta_{\nu\nu'} \delta_{mm'} \delta_{\kappa\kappa'} \ . \tag{3-263}
$$

Method Two. Without using intrinsic quantum numbers: For a given (ν, m) find τ_ν linearly independent solutions to Eq. (3-252). After the orthogonalization procedure, they become $\psi_m^{(\nu)j}, j = 1, 2, \ldots, \tau_\nu$. The other components are again obtained using

$$\psi_{m'}^{(\nu)j} = F_{m'm}^{(\nu)}(R)\psi_m^{(\nu)j} \ . \tag{3-264}$$

Now the index j is merely an additional label rather than an intrinsic quantum number, and the τ_ν sets of irreducible bases are chosen freely apart from the orthogonalization requirement.

3.13.3. Non-canonical subgroup chains

Now let us assume that the physically needed group chain $G \supset G(s)$ is not canonical. Therefore the corresponding operator set $(C, C(s))$ is not in general a CSCO in irreducible spaces of G. In other words, the eigenvalue of $(C, C(s))$ is not in general sufficient to label uniquely an irreducible basis vector. The non–canonical subgroup chains which we often come across in physics are of the form $G \supset G_1 \times G_2 \supset G(s_1) \times G(s_2)$, where $G_i \supset G(s_i), i = 1, 2$ are canonical. Let $(C_i, C(s_i))$ be the CSCO–II of G_i. Now the operator set

$$(C, C(s)) = (C, C_1, C(s_1), C_2, C(s_2))$$

is not a CSCO–II of G. We use $\psi^{(\nu)\kappa}_{\beta,\mu_1 m_1 \mu_2 m_2}$ to designate an irreducible basis vector adapted to the following group chain,

$$\begin{array}{ccccccccc} G & \supset & G_1 & \times & G_2 & \supset & G(s_1) & \times & G(s_2), \quad \overline{G} \supset \overline{G}(s') \\ \nu & & \mu_1 & & \mu_2 & & m_1 & & m_2 \quad \nu \quad \kappa \end{array} ,$$

where the group chain $\overline{G} \supset \overline{G}(s')$ can be chosen as canonical for simplicity, and β is an additional quantum number whose range is equal to the number of times, $(\mu_1 \mu_2 \nu)$, that the irrep (μ_1, μ_2) of $G_1 \times G_2$ occurs in the irrep ν of G. The irreducible basis satisfies the eigenequations

$$\begin{pmatrix} C \\ C_1 \\ C(s_1) \\ C_2 \\ C(s_2) \\ \overline{C}(s') \end{pmatrix} \psi^{(\nu)\kappa}_{\beta,\mu_1 m_1 \mu_2 m_2} = \begin{pmatrix} \nu \\ \mu_1 \\ m_1 \\ \mu_2 \\ m_2 \\ \kappa \end{pmatrix} \psi^{(\nu)\kappa}_{\beta,\mu_1 m_1 \mu_2 m_2} , \tag{3-265a}$$

$$\kappa = \kappa_1, \kappa_2, \ldots, \kappa_{\tau_\nu} \ , \quad \beta = 1, 2, \ldots, (\mu_1 \mu_2 \nu) \ .$$

For a given $(\nu, \mu_1, m_1, \mu_2, m_2, \kappa)$, there are $(\mu_1 \mu_2 \nu)$ linearly independent solutions to (3-265), which can be orthogonalized with respect to the index β. We only need to get the solutions for a particular m_1 and m_2. The remaining components of the irreducible basis can be obtained by

$$\begin{aligned} \psi^{(\nu)\kappa}_{\beta,\mu_1 m_1' \mu_2 m_2} &= F^{(\nu_1)}_{m_1' m_1}(R_1)\ \psi^{(\nu)\kappa}_{\beta,\mu_1 m_1 \mu_2 m_2} \\ \psi^{(\nu)\kappa}_{\beta,\mu_1 m_1 \mu_2 m_2'} &= F^{(\nu_2)}_{m_2' m_2}(R_2)\ \psi^{(\nu)\kappa}_{\beta \mu_1 m_1 \mu_2 m_2} \ . \end{aligned} \tag{3-265b}$$

If the irrep (ν) of G occurs only once in the reducible space $\{\varphi_a\}$, then the equation for $\overline{C}(s')$ and the quantum number κ are redundant.

3.13.4. The projection operator method

Traditionally, the principal method for constructing an irreducible basis of a finite group is the projection operator method. The procedure for projecting out an irreducible basis from a reducible basis $\{\varphi_a\}$ can be summarized as follows.

1. Compute the characters χ_i of the reducible rep carried by $\{\varphi_a\}$.
2. Using (3-249b), find the multiplicity τ_ν.
3. Find the irreducible matrices $D^{(\nu)}(R)$ for those irreps for which $\tau_\nu \geq 1$.

4. Apply the projection operator $P^{(\nu)}_{mk}$, (3-222), to one of the reducible basis vectors, say φ_1. If the result is not zero, then by varying m while keeping ν and k fixed, we can find a set of irreducible basis $\psi^{(\nu)}_m$.

5. If $P^{(\nu)}_{mk}\varphi_1 = 0$, then we change k to another quantum number k', and repeat step 4. If $P^{(\nu)}_{mk}\varphi_1 = 0$, for all k, then we change φ_1 to φ_2, and repeat steps 4 and 5, until we find a set of irreducible basis $\psi^{(\nu)}_m$.

6. If $\tau_\nu > 1$, by varying the quantum number k, we can get τ_ν sets of linearly independent but usually not orthogonal irreducible bases.

The projection operator method in its original form suffers from several drawbacks:

1. There is no rule governing the choice of the quantum number k and the basis vector φ_1 on which the projection operator applies.

2. In the case $\tau_\nu > 1$, the irreducible bases obtained from the projections with different k are in general neither linearly independent, nor orthogonal. If τ_ν is large, it is tedious to pick out the linearly independent ones.

3. The irreducible matrices for all group elements must be known beforehand.

4. The procedure is laborious and become intractable for groups of larger order.

The EFM is simpler and especially suitable for computer calculation. With the EFM, we can obtain the $G \supset G(s)$ irreducible basis without any prior knowledge of the $G \supset G(s)$ irreps.

It should be pointed out that for point groups by using the double-coset factored projection operator (see Sec. 8.7.1), or especially the algebraic expression of the projection operator (Sec .8.5 and Sec. 8.7) the projection operator method can be greatly simplified and very powerful.

3.14. Irreducible Basis Vectors in a Non–Orthogonal Reducible Basis

In previous sections it is assumed that the reducible basis vectors $\varphi_a : a = 1, 2, \ldots, n$ are orthonormal. We now consider the more general case of non–orthogonal states with $\langle\varphi_a|\varphi_b\rangle = g_{ab}$. Regular and non-regular representations are discussed separately.

1. *Regular representation*

Suppose that Φ_0 is a state without any symmetry. Applying R_a to it we get g nonorthogonal basis vectors, $\varphi_a = R_a\Phi_0 : a = 1, 2, \ldots, g$. We can still use the same projection operator $P^{(\nu)k}_m$ shown in (3-222) to get irreducible basis vectors $\psi^{(\nu)k}_m = P^{(\nu)k}_m\Phi_0$. Using

$$\begin{aligned}\langle\psi^{(\nu)k}_m|\psi^{(\nu')k'}_{m'}\rangle &= \langle\Phi_0|(P^{(\nu)k}_m)^\dagger P^{(\nu')k'}_{m'}|\Phi_0\rangle \\ &= \left(\tfrac{h_\nu}{g}\right)^{-1/2}\delta_{\nu\nu'}\delta_{mm'}\langle\Phi_0|P^{(\nu)k'}_k|\Phi_0\rangle\ ,\end{aligned} \tag{3-266}$$

and the fact that $\langle\Phi_0|R_a|\Phi_0\rangle = \langle\varphi_1|\varphi_a\rangle \neq \delta_{1,a}$, we see that the irreducible basis vectors $\psi^{(\nu)k}_m$ remain orthogonal in the quantum numbers ν and m, but they are no longer normalized and no longer orthogonal in the intrinsic quantum number k. Therefore apart from these two points, the irreducible basis vectors in the orthonormal basis and non–orthogonal basis are the same. To obtain normalized and orthogonal (with respect to the quantum number k) irreducible basis vectors for the latter case we need use the Schmidt procedure.

As can be checked, the irreducible basis vectors of S_3 given in Table 3.9 remain valid if the single particle states $|\alpha\rangle, |\beta\rangle$, and $|\gamma\rangle$ are nonorthogonal.

2. *Non regular representation*

(i). Using the projection operator method

The result is the same as for the regular representation with k replaced by κ.

(ii). Using the EFM

According to Sec. 2.12.4, so long as the representation matrices of C and $C(s)$ in the non orthogonal basis are defined according to the definition (2-110a),

$$C\varphi_a = \sum_b D_{ba}(C)\varphi_b,\ C(s)\varphi_a = \sum_b D_{ba}\left(C(s)\right)\varphi_b,$$

the problem of seeking the eigenvectors of $C, C(s)$ in the non-orthogonal basis is the same as in an orthonormal basis.

Therefore the irreducible basis vectors $\psi_m^{(\nu)}$ of S_3 given in (3-82) and (3-90) are still valid when the single-particle states $|\alpha\rangle, |\beta\rangle$ are nonorthogonal.

3.15. Kronecker Product of Representations

3.15.1 Clebsch-Gordan series

Suppose that one has two sets of functions $\psi_{m_1}^{(\nu_1)}(x_1)(m_1 = 1, 2, \ldots, h_{\nu_1})$ and $\varphi_{m_2}^{(\nu_2)}(x_2)(m_2 = 1, 2, \ldots, h_{\nu_2})$ which carry the irreps ν_1 and ν_2 of a group G, respectively. The $h_{\nu_1} h_{\nu_2}$ products

$$|m_1 m_2\rangle = \psi_{m_1}^{(\nu_1)}(x_1)\varphi_{m_2}^{(\nu_2)}(x_2) \tag{3-267}$$

form a rep space of G,

$$\begin{aligned} R|m_1 m_2\rangle &= \psi_{m_1}^{(\nu_1)}(R^{-1}x_1)\varphi_{m_2}^{(\nu_2)}(R^{-1}x_2) \\ &= \sum_{m_1' m_2'} D_{m_1' m_1}^{(\nu_1)}(R) D_{m_2' m_2}^{(\nu_2)}(R)|m_1' m_2'\rangle \\ &= \sum_{m_1' m_2'} D_{m_1' m_2', m_1 m_2}^{(\nu_1 \times \nu_2)}(R)|m_1' m_2'\rangle \ , \end{aligned} \tag{3-268}$$

$$D_{m_1' m_2', m_1 m_2}^{(\nu_1 \times \nu_2)}(R) = \langle m_1' m_2'|R|m_1 m_2\rangle = D_{m_1' m_1}^{(\nu_1)}(R) D_{m_2' m_2}^{(\nu_2)}(R) \ . \tag{3-269}$$

This rep of G is called the *direct product rep* or *Kronecker product* of the irreps ν_1 and ν_2 and is denoted by $(\nu_1) \times (\nu_2)$. Equation (3-269) can be written as

$$D^{(\nu_1 \times \nu_2)} = D^{(\nu_1)} \otimes D^{(\nu_2)} \ , \tag{3-270}$$

where the symbol $\otimes$ indicates the direct product of matrices. The product rep in general can be reduced into irreps of G,

$$D^{(\nu_1 \times \nu_2)} = \sum_{\nu_3} (\nu_1 \nu_2 \nu_3) D^{(\nu_3)} \ , \tag{3-271}$$

where $(\nu_1 \nu_2 \nu_3)$ is the number of times that the irrep ν_3 occurs in the product rep. Eq.(3-271) is referred to as the Clebsch-Gordan (CG) series, and is often represented in an abbreviated form as,

$$(\nu_1) \times (\nu_2) = \sum_{\nu_3} (\nu_1 \nu_2 \nu_3)(\nu_3) \ . \tag{3-272}$$

From (3-269) it is easy to calculate the character of the product rep.

$$\begin{aligned} \chi^{(\nu_1 \times \nu_2)}(R) &= \sum_{m_1 m_2} D_{m_1 m_2, m_1 m_2}^{(\nu_1 \times \nu_2)}(R) \\ &= \sum_{m_1 m_2} D_{m_1 m_1}^{(\nu_1)}(R) D_{m_2 m_2}^{(\nu_2)}(R) \\ &= \chi^{(\nu_1)}(R)\chi^{(\nu_2)}(R) \ , \end{aligned} \tag{3-273a}$$

which can be decomposed into a sum of the primitive characters,

$$\chi^{(\nu_1)}(R)\chi^{(\nu_2)}(R) = \sum_{\nu_3} (\nu_1 \nu_2 \nu_3)\chi^{(\nu_3)}(R) \ . \tag{3-273b}$$

Using (3-249b) we get

$$(\nu_1 \nu_2 \nu_3) = \sum_i \frac{g_i}{g} \chi_i^{(\nu_1)} \chi_i^{(\nu_2)} \chi_i^{(\nu_3)*} \ . \tag{3-274}$$

It is clear that

$$(\nu_1\nu_2\nu_3) = (\nu_2\nu_1\nu_3) \ . \tag{3-275}$$

For groups with real characters, we have

$$(\nu_1\nu_2\nu_3) = (\nu_i\nu_j\nu_k) \ , \tag{3-276}$$

where (ijk) is any permutation of (123).

We say a group G is *simply reducible* if the Kronecker product of any two irreps of G contains each irrep no more than once. Therefore, for a simply reducible group, all the coefficients $(\nu_1\nu_2\nu_3) \leq 1$. The permutation groups S_3 and S_4, and the rotation group R_3 are all simply reducible.

3.15.2. Symmetrized and anti-symmetrized squares

It is easy to show that the product rep $(\nu_1) \times (\nu_2)$ can be reduced into a symmetric and an anti-symmetric product reps

$$(\nu) \times (\nu) = [(\nu) \times (\nu)]_s \oplus [(\nu) \times (\nu)]_a \ , \tag{3-277}$$

where $[(\nu_1) \times (\nu_2)]_s$ is called the *symmetric part of the square*, or simply the symmetric square. It has the basis

$$\Psi_{jl} = \frac{1}{\sqrt{2(1+\delta_{jl})}}(\psi_j^{(\nu)}\varphi_l^{(\nu)} + \psi_l^{(\nu)}\varphi_j^{(\nu)}), \quad j \leq l = 1, \ldots, h_\nu \ . \tag{3-278}$$

Its dimension is $\binom{h_\nu}{2} + h_\nu = \frac{1}{2}h_\nu(h_\nu + 1)$. The representation matrices are

$$D^{[(\nu)\times(\nu)]_s}_{ik,jl} = \frac{1}{\sqrt{(1+\delta_{ik})(1+\delta_{jl})}}[D^{(\nu)}_{ij}D^{(\nu)}_{kl} + D^{(\nu)}_{il}D^{(\nu)}_{kj}] \tag{3-279}$$

where $i \leq k$, and $j \leq l$. The other part of (3-277), $[(\nu_1) \times (\nu_2)]_a$ is called the *anti-symmetric part of the square*, or simply the anti-symmetric square. It has the basis

$$\Phi_{jl} = \frac{1}{\sqrt{2}}(\psi_j^{(\nu)}\varphi_l^{(\nu)} - \psi_l^{(\nu)}\varphi_j^{(\nu)}), \quad j < l = 1, \ldots, h_\nu \ . \tag{3-280}$$

Its dimension is $\binom{h_\nu}{2} = \frac{1}{2}h_\nu(h_\nu - 1)$. The representation matrices are

$$D^{[(\nu)\times(\nu)]_a}_{ik,jl} = D^{(\nu)}_{ij}D^{(\nu)}_{kl} - D^{(\nu)}_{il}D^{(\nu)}_{kj} \ , \tag{3-281}$$

where $i < k$ and $j < l$. Both the symmetric and anti-symmetric parts of the square are in general reducible reps of G.

Ex. 3.20. Show that $\chi^{[\nu_1\times\nu_2]_s}(R) = \frac{1}{2}[\chi(R)^2 + \chi(R^2)]$ and $\chi^{[\nu_1\times\nu_2]_a}(R) = \frac{1}{2}[\chi(R)^2 - \chi(R^2)]$.

3.16. The Clebsch–Gordan (CG) Coefficients

3.16.1. Definition and properties of the CG coefficients

To effect the reduction of (3-271), the product basis vectors of (3-267) need to be recombined into the $G \supset G(s)$ irreducible basis

$$\begin{aligned} \Psi^{(\nu)\tau}_m(x_1, x_2) &= \sum_{m_1 m_2} C^{(\nu)\tau,m}_{\nu_1 m_1, \nu_2 m_2}\psi^{(\nu_1)}_{m_1}(x_1)\varphi^{(\nu_2)}_{m_2}(x_2) \ , \\ &\tau = 1, 2, \ldots, (\nu_1\nu_2\nu) \ , \end{aligned} \tag{3-282}$$

where τ is called the *outer multiplicity label* and the $C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2}$ are called *CG coefficients* or *Wigner coefficients* . If $(\nu_1\nu_2\nu) = 1$, then the corresponding CG coefficient is said to be multiplicity free.

Notice that the subgroups $G(s_1), G(s_2)$ and $G(s)$ used to characterize the irreducible bases $\psi_{m_1}^{\nu_1}, \varphi_{m_2}^{\nu_2}$ and $\Psi_m^{(\nu)\tau}$ may be different from one another, or may be identical.

Since Eq. (3-282) is a transformation between two sets of orthonormal bases, the CG coefficients satisfy the unitarity relations

$$\sum_{m_1 m_2} (C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2})^* C^{(\nu')\tau',m'}_{\nu_1 m_1,\nu_2 m_2} = \delta_{\nu\nu'}\delta_{\tau\tau'}\delta_{mm'} , \tag{3-283}$$

$$\sum_{\nu\tau m} (C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2})^* C^{(\nu)\tau,m}_{\nu_1 m_1',\nu_2 m_2'} = \delta_{m_1 m_1'}\delta_{m_2 m_2'} . \tag{3-284}$$

Applying the group element R to the left–hand side of Eq. (3-282), we have

$$R\Psi_m^{(\nu)\tau} = \sum_{m'} D^{(\nu)}_{m'm}(R)\Psi_{m'}^{(\nu)\tau} = \sum_{\substack{m'\\ m_1' m_2'}} D^{(\nu)}_{m'm}(R) C^{(\nu)\tau,m'}_{\nu_1 m_1',\nu_2 m_2'} \psi_{m_1'}^{(\nu_1)} \varphi_{m_2'}^{(\nu_2)} . \tag{3-285}$$

On applying the same group element R to the right–hand side of (3-282), we find that

$$R \sum_{m_1 m_2} C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2} \psi_{m_1}^{(\nu_1)} \varphi_{m_2}^{(\nu_2)} = \sum_{\substack{m_1 m_2\\ m_1' m_2'}} C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2} D^{(\nu_1)}_{m_1' m_1}(R) D^{(\nu_2)}_{m_2' m_2}(R) \psi_{m_1'}^{(\nu_1)} \varphi_{m_2'}^{(\nu_2)} . \tag{3-286}$$

Since the product basis vectors are linearly independent, we have

$$\sum_{m'} C^{(\nu)\tau,m'}_{\nu_1 m_1',\nu_2 m_2'} D^{(\nu)}_{m'm}(R) = \sum_{m_1 m_2} C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2} D^{(\nu_1)}_{m_1' m_1}(R) D^{(\nu_2)}_{m_2' m_2}(R) . \tag{3-287}$$

Multiplying both sides of (3-287) by $(C^{(\nu)\tau,m}_{\nu_1 \overline{m}_1,\nu_2 \overline{m}_2})^*$, summing over ν, τ, and m, and using (3-284), one has

$$\sum_{\nu\tau m m'} (C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2})^* C^{(\nu)\tau,m'}_{\nu_1 m_1',\nu_2 m_2'} D^{(\nu)}_{m'm}(R) = D^{(\nu_1)}_{m_1' m_1}(R) D^{(\nu_2)}_{m_2' m_2}(R) . \tag{3-288a}$$

Multiplying both sides of (3-288a) by $D^{(\bar{\nu})*}_{\overline{m}'\overline{m}}(R)$, summing over R and using (3-200a), gives

$$\frac{1}{g}\sum_R D^{(\nu)*}_{m'm}(R) D^{(\nu_1)}_{m_1' m_1}(R) D^{(\nu_2)}_{m_2' m_2}(R) = \frac{1}{h_\nu}\sum_\tau (C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2})^* C^{(\nu)\tau,m'}_{\nu_1 m_1',\nu_2 m_2'} . \tag{3-288b}$$

When all the irreducible matrices are real, setting $m' = m, m_1' = m_1$ and $m_2' = m_2$ in (3-288b) gives

$$\frac{1}{g}\sum_R D^{(\nu)}_{mm}(R) D^{(\nu_1)}_{m_1 m_1}(R) D^{(\nu_2)}_{m_2 m_2}(R) = \frac{1}{h_\nu}\sum_\tau |C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2}|^2 . \tag{3-289}$$

We therefore obtain the symmetry relations

$$\sum_\tau |C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2}|^2/h_\nu = \sum_\tau |C^{(\nu_2)\tau,m_2}_{\nu_1 m_1,\nu m}|^2/h_{\nu_2} = \sum_\tau |C^{(\nu_1)\tau,m_1}_{\nu m,\nu_2 m_2}|^2/h_{\nu_1} . \tag{3-290}$$

When either ν_1 or ν_2 is the identity rep I, the CG coefficients are trivial. From

$$R(\psi_{m_1}^{(\nu_1)}\varphi^{(I)}) = (R\psi_{m_1}^{(\nu_1)})(R\varphi^{(I)}) = \sum_{m_1'} D^{(\nu_1)}_{m_1' m_1}(R)(\psi_{m_1'}^{(\nu_1)}\varphi^{(I)})$$

one sees that the product basis $\psi_{m_1}^{(\nu_1)}\varphi^{(I)}$ remains the $G \supset G(s_1)$ irreducible basis (ν_1, m_1). Therefore one obtains

$$C_{\nu_1 m_1, I}^{(\nu),m} = C_{I,\nu_1 m_1}^{(\nu),m} = \delta_{\nu\nu_1}\delta_{mm_1} \ . \tag{3-291}$$

3.16.2. The EFM for CG coefficients

The CG coefficients have wide applications in physics and there is an abundant literature devoted to this problem. The conventional methods for computing the CG coefficients are essentially the projection operator method and its variations. For an extensive review of the subject the reader is referred to the review article by Chen, Gao & Ma (1985). In the following we only discuss the EFM.

According to (3-252), $\Psi_m^{(\nu)\tau}$ satisfies the eigenequations

$$\begin{pmatrix} C \\ C(s) \end{pmatrix} \Psi_m^{(\nu)\tau} = \begin{pmatrix} \nu \\ m \end{pmatrix} \Psi_m^{(\nu)\tau} \ . \tag{3-292}$$

Inserting (3-282) into (3-292) and multiplying from the left by $\langle m_1' m_2'|$, we have

$$\sum_{m_1 m_2} \left(\left\langle m_1' m_2' \left| \begin{matrix} C \\ C(s) \end{matrix} \right| m_1 m_2 \right\rangle - \begin{pmatrix} \nu \\ m \end{pmatrix} \delta_{m_1 m_1'} \delta_{m_2 m_2'} \right) C_{\nu_1 m_1, \nu_2 m_2}^{(\nu)\tau, m} = 0 \ , \tag{3-293}$$

$$\tau = 1, 2, \ldots (\nu_1 \nu_2 \nu) \ .$$

This shows that CG coefficients result from a diagonalization of the representative matrix of the CSCO–II of G in the product basis. The matrix elements of a class operator C_i are given by

$$\langle m_1' m_2' | C_i | m_1 m_2 \rangle = \sum_{l=1}^{g_i} D_{m_1' m_1}^{(\nu_1)}(R_l^{(i)}) D_{m_2' m_2}^{(\nu_2)}(R_l^{(i)}) \ . \tag{3-294}$$

Notice that

$$\langle m_1' m_2' | C_i | m_1 m_2 \rangle \neq D_{m_1' m_1}^{(\nu_1)}(C_i) D_{m_2' m_2}^{(\nu_2)}(C_i) \ .$$

Using (3-294) we can calculate the matrix elements of the CSCO-II. From the characteristic equation (3-293), we can obtain the eigenvalue (ν, m) along with its degeneracy, which gives the multiplicity $(\nu_1 \nu_2 \nu)$ in the CG series (3-272).

When $(\nu_1 \nu_2 \nu) > 1$, for a given (ν, m), there are $(\nu_1 \nu_2 \nu)$ sets of linearly independent solutions to Eq. (3-293). Subject to the orthogonality requirement with respect to the multiplicity label τ, that is

$$\begin{gathered} \langle \Psi_m^{(\nu)\tau} | \Psi_m^{(\nu)\tau'} \rangle = \delta_{\tau\tau'}, \\ \sum_{m_1 m_2} (C_{\nu_1 m_1, \nu_2 m_2}^{(\nu)\tau, m})^* C_{\nu_1 m_1, \nu_2 m_2}^{(\nu)\tau', m} = \delta_{\tau\tau'} \ , \end{gathered} \tag{3-295}$$

the $(\nu_1 \nu_2 \nu)$ sets of solutions can be chosen arbitrarily.

For each possible ν we only take the CG coefficients for a particular m from (3-293); the remaining CG coefficients of the irrep (ν) should be evaluated with the help of (3-264), that is using

$$C_{\nu_1 m_1', \nu_2 m_2'}^{(\nu)\tau, m'} = \sum_{m_1 m_2} \langle m_1' m_2' | F_{m' m}^{(\nu)}(R) | m_1 m_2 \rangle C_{\nu_1 m_1, \nu_2 m_2}^{(\nu)\tau, m} \ . \tag{3-296}$$

It is to be noted that the multiplicity separation is arbitrary, and that the following linear combination satisfies all our requirements for the CG coefficient,

$$C_{\nu_1 m_1, \nu_2 m_2}^{(\nu)\theta, m} = \sum_{\tau} S_{\theta\tau}^{(\nu)} C_{\nu_1 m_1, \nu_2 m_2}^{(\nu)\tau, m} \ , \tag{3-297}$$

where $S^{(\nu)}$ is a $(\nu_1 \nu_2 \nu) \times (\nu_1 \nu_2 \nu)$ unitary matrix. Hence the CG coefficient can be determined only up to a unitary transformation.

The advantage of the EFM for calculating the CG coefficients is that only the irreducible matrices of a few group elements (which are contained in the CSCO–II of G) are required, while in the projection operator method, the irreducible matrices of all the $|G|$ group elements are required. Another feature of the EFM is that the CG series and CG coefficients are obtained simultaneously.

3.17. Isoscalar Factors

The question we address in this section is; How can we find the CG coefficients for the $G \supset G_1 \supset G_1(s)$ irreducible basis when the CG coefficients for the $G_1 \supset G_1(s)$ irreducible basis are known?

The CG coefficients for the $G_1 \supset G_1(s)$ irreducible basis are defined through

$$|\Lambda_\theta, m\rangle = \sum_{m_1 m_2} C^{(\Lambda)\theta,m}_{\Lambda_1 m_1, \Lambda_2 m_2} |\Lambda_1 m_1\rangle |\Lambda_2 m_2\rangle \ , \qquad \theta = 1, 2, \ldots (\Lambda_1 \Lambda_2 \Lambda), \tag{3-298}$$

where θ is the outer multiplicity label for the group G_1.

The $G \supset G_1 \supset G_1(s)$ irreducible basis is designated $\left|{}^{(\nu)\tau}_{\beta\Lambda m}\right\rangle$, where β $(= 1, 2, \ldots a_\Lambda)$ is the *inner multiplicity* which takes account of the multiple occurrence of the irrep Λ of G_1 in the irrep ν of G,

$$D^{(\nu)} = \sum_\Lambda \oplus a_\Lambda D^{(\Lambda)} \ , \tag{3-299}$$

The CG coefficients for the $G \supset G_1 \supset G_1(s)$ irreducible basis are defined through

$$\left|{}^{(\nu)\tau}_{\beta\Lambda m}\right\rangle = \sum_{\substack{\beta_1\Lambda_1 m_1 \\ \beta_2\Lambda_2 m_2}} C^{(\nu)\tau,\beta\Lambda m}_{\nu_1\beta_1\Lambda_1 m_1, \nu_2\beta_2\Lambda_2 m_2} \left|{}^{(\nu_1)}_{\beta_1\Lambda_1 m_1}\right\rangle \left|{}^{(\nu_2)}_{\beta_2\Lambda_2 m_2}\right\rangle \ , \qquad \tau = 1, 2, \ldots (\nu_1\nu_2\nu) \ . \tag{3-300}$$

An alternative way for constructing the $G \supset G_1 \supset G_1(s)$ irreducible basis in (3-300) is to first use the $G_1 \supset G_1(s)$ CG coefficients to couple $\left|{}^{(\nu_1)}_{\beta_1\Lambda_1 m_1}\right\rangle$ and $\left|{}^{(\nu_2)}_{\beta_2\Lambda_2 m_2}\right\rangle$ into the irreducible basis $|\Lambda_\theta, m\rangle$ of G_1, that is

$$\left[\left|{}^{(\nu_1)}_{\beta_1\Lambda_1}\right\rangle \left|{}^{(\nu_2)}_{\beta_2\Lambda_2}\right\rangle\right]^{\Lambda_\theta}_m = \sum_{m_1 m_2} C^{(\Lambda)\theta,m}_{\Lambda_1 m_1, \Lambda_2 m_2} \left|{}^{(\nu_1)}_{\beta_1\Lambda_1 m_1}\right\rangle \left|{}^{(\nu_1)}_{\beta_2\Lambda_2 m_2}\right\rangle \ , \tag{3-301}$$

and then using the so–called $G \supset G_1$ *isoscalar factor* (ISF), or the *reduced Wigner coefficients*, $C^{(\nu)\tau,\beta\Lambda_\theta}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2}$, to combine (3-301) into the irreducible basis of G,

$$\left|{}^{(\nu)\tau}_{\beta\Lambda m}\right\rangle = \sum_{\beta_1\Lambda_1\beta_2\Lambda_2\theta} C^{(\nu)\tau,\beta\Lambda_\theta}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2} \left[\left|{}^{(\nu_1)}_{\beta_1\Lambda_1}\right\rangle \left|{}^{(\nu_2)}_{\beta_2\Lambda_2}\right\rangle\right]^{\Lambda_\theta}_m \ . \tag{3-302}$$

From Eqs. (3-300)-(3-302) one has

$$C^{(\nu)\tau,\beta\Lambda m}_{\nu_1\beta_1\Lambda_1 m_1,\nu_2\beta_2\Lambda_2 m_2} = \sum_\theta C^{(\nu)\tau,\beta\Lambda_\theta}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2} C^{(\Lambda)\theta,m}_{\Lambda_1 m_1,\Lambda_2 m_2} \ . \tag{3-303}$$

This is the celebrated *Racah Factorization Lemma.* It tells us that from the $G \supset G_1$ ISF and $G_1 \supset G_1(s)$ CG coefficients, we can easily construct the $G \supset G_1 \supset G_1(s)$ CG coefficients. Equation (3-303) is also valid for Lie groups.

Racah's Lemma can be applied to any link in the group chain. For example, the CG coefficients for the group chain $G \supset G_1 \supset G_2 \supset G_3$ can be expressed schematically as

$$(G \supset G_1 \supset G_2 \supset G_3)_{CGC} = (G \supset G_1)_{\text{ISF}} \times (G_1 \supset G_2)_{\text{ISF}} \times (G_2 \supset G_3)_{\text{CGC}} \tag{3-304}$$

Therefore, the calculation of the CG coefficients for a large group G is reduced to the computation of the ISF in each link of the group chain starting from the group G.

Equation (3-302) represents a similarity transformation between two sets of orthonormal bases, therefore the ISF satisfy the unitarity relations

$$\sum_{\substack{\beta_1\Lambda_1\theta \\ \beta_2\Lambda_2}} (C^{(\nu)\tau,\beta\Lambda_\theta}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2})^* C^{(\nu')\tau',\beta'\Lambda_\theta}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2} = \delta_{\nu\nu'}\delta_{\tau\tau'}\delta_{\beta\beta'} , \tag{3-305}$$

$$\sum_{\nu\tau\beta} (C^{(\nu)\tau,\beta\Lambda_\theta}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2})^* C^{(\nu)\tau,\beta\Lambda_{\theta'}}_{\nu_1\beta_1'\Lambda_1',\nu_2\beta_2'\Lambda_2'} = \delta_{\beta_1\beta_1'}\delta_{\beta_2\beta_2'}\delta_{\Lambda_1\Lambda_1'}\delta_{\Lambda_2\Lambda_2'}\delta_{\theta\theta'} . \tag{3-306}$$

Note that the quantum number Λ is kept fixed in the above equations.

The inverse of (3-302) is

$$\left[\left|\begin{matrix}(\nu_1)\\ \beta_1\Lambda_1\end{matrix}\right\rangle \left|\begin{matrix}(\nu_2)\\ \beta_2\Lambda_2\end{matrix}\right\rangle\right]^{\Lambda_\theta}_m = \sum_{\nu\tau\beta} (C^{(\nu)\tau,\beta\Lambda_\theta}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2})^* \left|\begin{matrix}(\nu)_\tau\\ \beta\Lambda m\end{matrix}\right\rangle . \tag{3-307}$$

The EFM for the ISF will be further discussed in Secs. 4.19, 7.16 and 7.17.

The CG coefficients discussed in this book are all real except those for the space groups. For the real CG coefficients, we omit the complex conjugate symbol *.

3.18. Irreducible Tensors for a Group G

3.18.1. The definition of an irreducible tensor

We say that a collection of operators

$$T^{(\nu)}_m,\ m = 1, 2, \ldots, h_\nu \tag{3-308a}$$

is a set of irreducible tensors of a group G, if under the action of the group G it transforms as

$$RT^{(\nu)}_m R^{-1} = \sum_{m'} D^{(\nu)}_{m'm}(R) T^{(\nu)}_{m'} . \tag{3-308b}$$

Equivalently we say that $T^{(\nu)}_m$ is the m–th component of the ν–th irreducible tensor of G.

If an operator H is invariant under the group G,

$$RHR^{-1} = H ,$$

or written as

$$[H, R] = 0 , \quad R \in G , \tag{3-309}$$

then H is called a *scalar operator* of the group G, or an *invariant* of G, or an *irreducible tensor* of the identity rep.

The EFM can also be used to construct irreducible tensors. For example, from the one–body operators, $O_i, i = 1, 2, 3$, we can construct the following irreducible tensors of the permutation group S_3,

$$O^{(3)} = \sqrt{\tfrac{1}{3}}(O_1 + O_2 + O_3), \quad O^{(0)}_1 = \sqrt{\tfrac{1}{6}}(O_1 + O_2 - 2O_3), \quad O^{(0)}_{-1} = \sqrt{\tfrac{1}{2}}(O_1 - O_2) . \tag{3-310a}$$

Similarly, for the two-body operators O_{ij}, we can obtain the irreducible tensor of S_3,

$$O^{(3)} = \sqrt{\tfrac{1}{3}}(O_{12}+O_{13}+O_{23}),\ O_1^{(0)} = \sqrt{\tfrac{1}{6}}(2O_{12}-O_{13}-O_{23}),\ O_{-1}^{(0)} = \sqrt{\tfrac{1}{2}}(O_{13}-O_{23}). \tag{3-310b}$$

By means of the CG coefficients, two irreducible tensors $T^{(\nu_1)}$ and $U^{(\nu_2)}$ of the group G can be coupled into another irreducible tensor $V^{(\nu)}$:

$$V_m^{(\nu)\tau} = \sum_{m_1 m_2} C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2} T^{(\nu_1)}_{m_1} U^{(\nu_2)}_{m_2}\ . \tag{3-311a}$$

To see this, note that

$$\begin{aligned} RV_m^{(\nu)\tau}R^{-1} &= \sum_{m_1 m_2} C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2} RT^{(\nu_1)}_{m_1}R^{-1}RU^{(\nu_2)}_{m_2}R^{-1} \\ &= \sum_{m_1 m_2 m_1' m_2'} C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2} D^{(\nu_1)}_{m_1' m_1}(R) D^{(\nu_2)}_{m_2' m_2}(R) T^{(\nu_1)}_{m_1'} U^{(\nu_2)}_{m_2'} \\ &= \sum_{m' m_1' m_2'} D^{(\nu)}_{m' m}(R) C^{(\nu)\tau,m'}_{\nu_1 m_1',\nu_2 m_2'} T^{(\nu_1)}_{m_1'} U^{(\nu_2)}_{m_2'} \\ &= \sum_{m'} D^{(\nu)}_{m' m}(R) V_{m'}^{(\nu)\tau}\ , \end{aligned} \tag{3-311b}$$

where Eq. (3-287) has been used.

The most familiar example of an irreducible tensor is the spherical harmonic $Y_{lm}, m = -l,\ldots,l$, which is an irreducible tensor of the rotation group R_3.

3.18.2. Two kinds of invariants

There are two kinds of invariants, denoted as C and M, of a group G.

$$\begin{aligned} &[C,G]=0,\ C\in L_g, \\ &[M,G]=0,\ M\notin L_g, \end{aligned} \tag{3-312a}$$

where L_g is the group algebra of G. The operators C and M are called the first and second kind of invariants of G, respectively. For example a class operator is a first kind of invariants, while a Hamiltonian with G as its symmetry group is in general a second kind of invariants. Another example is that in the regular rep space the intrinsic operator $\bar{C}(s)$ is of the second kind of invariants.

Since M commutes with any element of G, it commutes necessarily with C,

$$[C,M]=0. \tag{3-312b}$$

Suppose that in a representation space an irrep (ν) occurs τ_ν times. Let $\psi_m^{(\nu)\tau}$ be a basis vector of the τ-th irrep (ν) of G, $\tau = 1,2,\ldots,\tau_\nu$. Under the operation of C and M, $\psi_m^{(\nu)\tau}$ transforms as

$$C\psi_m^{(\nu)\tau} = \lambda^\nu \psi_m^{(\nu)\tau},\ \tau = 1,2,...,\tau_\nu, \tag{3-312c}$$

$$M\psi_m^{(\nu)\tau} = \sum_{\tau'=1}^{\tau_\nu} M_{\tau'\tau}\psi_m^{(\nu)\tau'}. \tag{3-312d}$$

Namely, $\psi_m^{(\nu)\tau}$ is necessarily an eigenvector of C, but is in general not an eigenvector of M. If $\tau_\nu > 1$, the τ_ν basis vectors $\psi_m^{(\nu)\tau}$ can be combined linearly into eigenvectors of the operator M,

$$M\Psi_m^{(\nu)\mu} = \mu\Psi_m^{(\nu)\mu}. \tag{3-312e}$$

The eigenvalue μ now serves as the multiplicity label for the τ_ν equivalent irreps ν of G (If μ has degeneracy, then the labelling is not unique). Therefore the second kind of invariants M is called the *multiplicity operator* of G . In the case of $\tau_\nu = 1$, (3-312e) reduces to

$$M\psi_m^{(\nu)} = \mu\psi_m^{(\nu)},$$

that is, for a multiplicity free case the irreducible basis vector $\psi_m^{(\nu)}$ is also an eigenvector of the multiplicity operator M.

3.18.3. The Wigner–Eckart theorem

In analogy with Eq. (3-311b) we can prove that

$$\varphi_{m_2'}^{(\nu_2')\tau} = \sum_{mm_1} C_{\nu_1 m_1, \nu m}^{(\nu_2')\tau, m_2'} T_m^{(\nu)} \psi_{m_1}^{(\nu_1)} \tag{3-313}$$

is again an irreducible basis of G. The inverse is

$$T_m^{(\nu)} \psi_{m_1}^{(\nu_1)} = \sum_{\nu_2' m_2' \tau} \left(C_{\nu_1 m_1, \nu m}^{(\nu_2')\tau, m_2'}\right)^* \varphi_{m_2'}^{(\nu_2')\tau} \ . \tag{3-314}$$

Using (3-314), the matrix element of $T_m^{(\nu)}$ can be expressed as

$$\langle \psi_{m_2}^{(\nu_2)} | T_m^{(\nu)} | \psi_{m_1}^{(\nu_1)} \rangle = \sum_{\nu_2' m_2' \tau} \left(C_{\nu_1 m_1, \nu m}^{(\nu_2')\tau, m_2'}\right)^* \langle \psi_{m_2}^{(\nu_2)} | \varphi_{m_2'}^{(\nu_2')\tau} \rangle \ . \tag{3-315}$$

According to Schur's Lemma (2-108), we have

$$\langle \psi_{m_2}^{(\nu_2)} | \varphi_{m_2'}^{(\nu_2')\tau} \rangle = \langle \psi_{m_2}^{(\nu_2)} | 1 | \varphi_{m_2'}^{(\nu_2')\tau} \rangle = \text{const.}\, \delta_{\nu_2 \nu_2'} \cdot \delta_{m_2 m_2'} \ , \tag{3-316a}$$

where the constant is independent of m and m', is a function of ν_1, ν_2, ν and τ, and is denoted by

$$\langle \psi^{(\nu_2)} \, \| T^{(\nu)} \| \, \psi^{(\nu_1)} \rangle_G^{(\tau)} \tag{3-316b}$$

and called the reduced matrix element with respect to the group G, or the *G– reduced matrix element* , or simply the *reduced matrix element* if no confusion arises, and the notation is shortened as

$$\langle \psi^{(\nu_2)} \, \| T^{(\nu)} \| \, \psi^{(\nu_1)} \rangle^{(\tau)}. \tag{3-316c}$$

We follow the definition in Rose (1957) which is related to the Edmonds' (1957) definition by

$$\langle \psi^{(\nu_2)} \, \| T^{(\nu)} \| \, \psi^{(\nu_1)} \rangle = \sqrt{\frac{1}{h_{\nu_2}}} \langle \psi^{(\nu_2)} \, \| T^{(\nu)} \| \, \psi^{(\nu_1)} \rangle_{\text{Edmonds}} \ .$$

From (3-315) and (3-316) we obtain the celebrated *Wigner–Eckart Theorem*,

$$\langle \psi_{m_2}^{(\nu_2)} | T_m^{(\nu)} | \psi_{m_1}^{(\nu_1)} \rangle = \sum_{\tau} \left(C_{\nu_1 m_1, \nu m}^{(\nu_2)\tau, m_2}\right)^* \langle \psi^{(\nu_2)} \| \, T^{(\nu)} \| \psi^{(\nu_1)} \rangle^{\tau} \ . \tag{3-317}$$

The inverse of (3-317) gives the irreducible matrix element

$$\langle \psi^{(\nu_2)} \, \| T^{(\nu)} \| \, \psi^{(\nu_1)} \rangle^{(\tau)} = (-1)^{\nu_2 - \nu - \nu_1} \left\langle \psi_{m_2}^{(\nu_2)} \middle| \left(T^{(\nu)} \psi^{(\nu_1)}\right)_{m_2}^{(\nu_2)\tau} \right\rangle \ . \tag{3-318}$$

According to the Wigner–Eckart Theorem, the matrix element of an irreducible tensor is expressible in terms of a sum of products of two factors, one is a symmetry–related geometric factor, the CG coefficient, and the other is a physical factor, the reduced matrix element. The

specific properties of the states and the operator enter the physical factor only. It is precisely this that makes the Wigner–Eckart Theorem invaluable in physics. The Wigner–Eckart Theorem is also applicable to compact Lie groups.

For simply reducible groups, the multiplicity index τ is redundant, and (3-317) reduces to

$$\langle \psi^{(\nu_2)}_{m_2} | T^{(\nu)}_m | \psi^{(\nu_1)}_{m_1} \rangle = \left(C^{\nu_2, m_2}_{\nu_1 m_1, \nu m} \right)^* \langle \psi^{(\nu_2)} \| T^{(\nu)} \| \psi^{(\nu_1)} \rangle \ , \tag{3-319a}$$

showing that the matrix element is factorizable.

If $T^{(\nu)}$ is an invariant operator H of the group G, letting $\nu = I$ (the identity rep) in (3-319a) we have

$$\langle \psi^{(\nu_2)}_{m_2} | H | \psi^{(\nu_1)}_{m_1} \rangle = \delta_{\nu_1 \nu_2} \delta_{m_1 m_2} \langle \psi^{(\nu_1)} \| H \| \psi^{(\nu_1)} \rangle \ , \tag{3-319b}$$

which says that an invariant has zero matrix elements between any two non-equivalent irreps and that within an irrep it is diagonal. Thus we retrieve Schur's Lemma (2-108). Notice that an invariant of the second kind has non-vanishing matrix elements between two equivalent irreps (see Eq. (3-312d)).

The above discussion on the reduced matrix elements can be extended to subgroup chain symmetry adapted bases. Let $\psi^{(\nu)}_{\Lambda m}$ be the $G \supset G_1 \supset G_1(s)$ irreducible basis. Using the Wigner-Eckart Theorem with respect to the groups G and G_1 we have

$$\begin{aligned} \langle \psi^{(\nu_2)}_{\Lambda_2 m_2} | T^{(\nu)}_{\Lambda m} | \psi^{(\nu_1)}_{\Lambda_1 m_1} \rangle &= \sum_{\tau} \left(C^{(\nu_2)\tau, \Lambda_2 m_2}_{\nu_1 \Lambda_1 m_1, \nu \Lambda m} \right)^* \langle \psi^{(\nu_2)} \| T^{(\nu)} \| \psi^{(\nu_1)} \rangle^{\tau}_{G} \\ &= \sum_{\theta} \left(C^{(\Lambda_2)\theta, m_2}_{\Lambda_1 m_1, \Lambda m} \right)^* \langle \psi^{(\nu_2)}_{\Lambda_2} \| T^{(\nu)}_{\Lambda} \| \psi^{(\nu_1)}_{\Lambda_1} \rangle^{\theta}_{G_1} \ . \end{aligned}$$

In Wybourne (1979) the matrix elements $\langle \ \| \ \| \ \rangle_{G_1}$ and $\langle \ \| \ \| \ \rangle_{G}$ are called the *singly* and *doubly reduced matrix elements*, respectively .

Using (3-303) we get the relation between the singly and doubly reduced matrix elements,

$$\langle \psi^{(\nu_2)}_{\Lambda_2} \| T^{(\nu)}_{\Lambda} \| \psi^{(\nu_1)}_{\Lambda_1} \rangle^{\theta}_{G_1} = \sum_{\tau} \langle \psi^{(\nu_2)} \| T^{(\nu)} \| \psi^{(\nu_1)} \rangle^{\tau}_{G} \left(C^{(\nu_2)_\tau, (\Lambda_2)_\theta}_{\nu_1 \Lambda_1, \nu \Lambda} \right)^* \ . \tag{3-320}$$

Namely,

$$(G_1\text{–r.m.e.}) = (G\text{–r.m.e.})(G \supset G_1 \ \text{ISF})^* .$$

Expositions on irreducible tensors for point groups and permutation groups have been given by Griffith (1962) and Vanagas (1972).

3.19. Symmetries of the CG Coefficients and Isoscalar Factors

The CG coefficients and ISF have many symmetries (see Hamermesh 1962, Derome 1966, Wybourne 1974, Butler 1975, Gao & Chen 1985). The labor involved in the computation of these coefficients can be greatly reduced by considering their symmetry properties with respect to the permutation of their arguments and their relation to complex conjugate reps.

1. Since the CG series for $(\nu_1) \times (\nu_2)$ and $(\nu_2) \times (\nu_1)$ are identical, we must have

$$C^{(\nu)\tau, m}_{\nu_1 m_1, \nu_2 m_2} = \varepsilon_1 C^{(\nu)\tau, m}_{\nu_2 m_2, \nu_1 m_1} \ , \tag{3-321}$$

where $\varepsilon_1 = \varepsilon_1(\nu_1 \nu_2 \nu_\tau)$ is a phase factor. For $\nu_1 \neq \nu_2$, the factor is determined by the phase convention. For $\nu_1 = \nu_2$, $\varepsilon_1 = 1$ if ν belongs to the symmetric square, and $\varepsilon_1 = -1$ if ν_τ belongs to the anti–symmetric square.

2. We use $(\overline{\nu})$ and $(\overline{m})$ to denote the contragredient reps of G and $G(s)$. For unitary reps we have

$$D^{(\overline{\nu})}_{\overline{m}' \overline{m}}(R) = D^{(\nu)*}_{m' m}(R) \ . \tag{3-322}$$

Taking the complex conjugate of (3-287) and making use of Eq. (3-322), we obtain a second symmetry relation

$$C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2} = \varepsilon_2 \big(C^{(\overline{\nu})\tau,\overline{m}}_{\overline{\nu}_1 \overline{m}_1,\overline{\nu}_2 \overline{m}_2}\big)^* , \tag{3-323}$$

where $\varepsilon_2 = \varepsilon_2(\nu_1 \nu_2 \nu_\tau)$ is a phase factor.

3. From the Hermitian conjugate of (3-308b) one has

$$R T^{(\nu)\dagger}_m R^{-1} = \sum_{m'} D^{(\nu)^*}_{m'm}(R) T^{(\nu)\dagger}_{m'} .$$

This shows that $T^{(\nu)^\dagger}_m$ transforms contragrediently to $T^{(\nu)}_m$, that is

$$T^{(\nu)^\dagger}_m = T^{(\overline{\nu})}_{\overline{m}} . \tag{3-324a}$$

Therefore one obtains

$$\langle \nu_1 m_1 | T^{(\nu)}_m | \nu_2 m_2 \rangle = \langle \nu_1 m_1 | T^{(\overline{\nu})^\dagger}_{\overline{m}} | \nu_2 m_2 \rangle . \tag{3-324b}$$

Let us first assume that the Kronecker products $(\nu) \times (\nu_1)$ and $(\nu) \times (\nu_2)$ are simply reducible. From our last result and the Wigner–Eckart Theorem (3-319) we obtain

$$(C^{\nu_1,m_1}_{\nu m,\nu_2 m_2})^* \langle \nu_1 \, \| T^{(\nu)} \| \, \nu_2 \rangle = C^{\nu_2,m_2}_{\overline{\nu}\,\overline{m},\nu_1 m_1} \langle \nu_2 \, \| T^{(\overline{\nu})} \| \, \nu_1 \rangle^* . \tag{3-325}$$

Squaring, summing over m_1, m_2 and m, and using the orthogonality of the CG coefficients, we have

$$\sqrt{h_{\nu_1}} |\langle \nu_1 \, \| T^{(\nu)} \| \, \nu_2 \rangle| = \sqrt{h_{\nu_2}} |\langle \nu_2 \, \| T^{(\overline{\nu})} \| \, \nu_1 \rangle| . \tag{3-326a}$$

On substituting (3-326a) into (3-325) and using (3-323) and (3-321) we obtain another symmetry relation

$$\sqrt{\frac{1}{h_\nu}} C^{(\nu),m}_{\nu_1 m_1,\nu_2 m_2} = \varepsilon_3 \sqrt{\frac{1}{h_{\nu_1}}} C^{(\overline{\nu}_1),\overline{m}_1}_{\overline{\nu}\,\overline{m},\nu_2 m_2} . \tag{3-327a}$$

If the multiplicity is larger than 1, then (3-326a) is replaced by

$$h_{\nu_1} \sum_\tau |\langle \nu_1 \, \| T^{(\nu)} \| \, \nu_2 \rangle^{(\tau)}|^2 = h_{\nu_2} \sum_\tau |\langle \nu_2 \, \| T^{(\overline{\nu})} \| \, \nu_1 \rangle^{(\tau)}|^2 , \tag{3-326b}$$

and (3-327a) is no longer true in general.

In the case when all the irreps of a group G are real, the CG coefficients obey Eq. (3-290). Through suitable linear combinations (Hamermesh 1962), the CG coefficients can be made to satisfy the following symmetry

$$\sqrt{\frac{1}{h_\nu}} C^{(\nu)\tau,m}_{\nu_1 m_1,\nu_2 m_2} = \varepsilon_3' \sqrt{\frac{1}{h_{\nu_1}}} C^{(\nu_1)\tau,m_1}_{\nu m,\nu_2 m_2} . \tag{3-327b}$$

From the symmetries of the CG coefficients, we obtain the symmetries of the ISF:

$$C^{(\nu)\tau,\beta\Lambda_\theta}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2} = \eta_1 C^{(\nu)\tau,\beta\Lambda_\theta}_{\nu_2\beta_2\Lambda_2,\nu_1\beta_1\Lambda_1} . \tag{3-328}$$

When $\nu_1 \neq \nu_2$, the phase factor η_1 is determined by the phase convention.

2. If the multiplicity label θ is redundant, from Eqs. (3-323) and (3-303) we have

$$C^{(\nu)\tau,\beta\Lambda}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2} = \eta_2 (C^{(\overline{\nu})\tau,\beta\overline{\Lambda}}_{\overline{\nu}_1\beta_1\overline{\Lambda}_1,\overline{\nu}_2\beta_2\overline{\Lambda}_2})^* . \tag{3-329}$$

3. When both the multiplicity labels τ and θ are redundant,

$$\sqrt{\frac{h_\Lambda}{h_\nu}} C^{(\nu),\beta\Lambda}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2} = \eta_3 \sqrt{\frac{h_{\Lambda_1}}{h_{\nu_1}}} C^{(\overline{\nu}_1),\beta_1\overline{\Lambda}_1}_{\overline{\nu}\beta\overline{\Lambda},\nu_2\beta_2,\Lambda_2} . \tag{3-330a}$$

4. When all the irreps are real,

$$\sqrt{\frac{h_\Lambda}{h_\nu}}C^{(\nu)\tau,\beta\Lambda\theta}_{\nu_1\beta_1\Lambda_1,\nu_2\beta_2\Lambda_2} = \eta'_3\sqrt{\frac{h_{\Lambda_1}}{h_{\nu_1}}}C^{(\nu_1)\tau,\beta_1\Lambda_1\theta}_{\nu\beta\Lambda,\nu_2\beta_2\Lambda_2} . \tag{3-330b}$$

Remark: For the multiplicity–free case, the symmetries (3-321), (3-323) and (3-327b), or equivalently, (3-328), (3-329) and (3-330b), are satisfied automatically. For non–multiplicity–free cases, the above symmetries can be imposed to reduce the arbitrariness in the multiplicity separation.

3.20. Applications of Group Theory in Quantum Mechanics

Modern developments in all branches of physics are putting more and more emphasis on the role of symmetries of the underlying physical systems. The application of group theory in quantum mechanics is diversifying, and is a central subject in numerous books (Lobel 1968, 1971, 1975, Bacry 1977, Elliott & Dawber 1979, Biedenharn & Louck 1981, Tung 1985, Stancu 1996, Inui, 1996, Cornwell 1997, Fuchs 1997). In this section, we sketch some key points.

3.20.1. When G is the symmetry group of the Hamiltonian

1. *State–labelling problem.*

To give a state we must first name it, to distinguish if form the others. This is the state–labelling problem, that of finding a complete set of labels, which fix the state vector of the system. Now we have a simple answer to this question. Since $[H, G] = 0$, we have

$$[H, C] = 0, \quad [H, C(s)] = 0 , \tag{3-331}$$

so that C and $C(s)$ are constants of motion. Therefore the eigenvalues (ν, m) of the CSCO–II of $G, (C, C(s))$, are good quantum numbers and can be used to label, though not uniquely, the energy level of the system. The set of operators $\big(H, C, C(s)\big)$ usually provides a complete set of labels (E, ν, m) for eigenstates of the system. For example, for hydrogen atom the set of eigenvalues $\big(E, l(l+1), l_z\big)$ of $\big(H, \mathbf{L}^2, L_z\big)$, or (n, l, m) is a complete set of labels, where n is the principal quantum number.

It should be noted that in the standard representation theory, the irreps of finite groups are labelled by primitive characters or some special symbols, such as the Young diagram for permutation group and unitary group, the Mulliken notation for point groups (Sec. 8.3.1), etc. instead of eigenvalues of some operators. Using the eigenvalue of the CSCO of G as irrep label immediately narrows the gap between group theory and quantum mechanics.

2. *Simplifying the problem of solving the Schrödinger equation.*

Suppose that $\{\varphi_a : a = 1, 2, \ldots, n\}$ carries a rep $\mathcal{D}$ for both the Hamiltonian H and its symmetry group G,

$$\mathcal{D}_{ab}(H) = \langle\varphi_a|H|\varphi_b\rangle , \tag{3-332a}$$

$$\mathcal{D}_{ab}(R) = \langle\varphi_a|R|\varphi_b\rangle, \quad \text{for } R \in G . \tag{3-332b}$$

The energies of the system are decided upon by the expectation equation

$$\det|\mathcal{D}(H) - E\,I|_1^n = 0 . \tag{3-332c}$$

Instead of directly solving Eq. (3-332c), we first find the irreducible basis of the symmetry group G,

$$\psi_m^{(\nu)\kappa} = \sum_{a=1}^{n} a_{m,a}^{(\nu)\kappa}\varphi_a, \quad m = 1, 2, \ldots, h_\nu, \quad \kappa = 1, 2, \ldots, \tau_\nu , \tag{3-332d}$$

$$n = \sum_{\nu=1}^{N} \tau_\nu h_\nu . \tag{3-332e}$$

In the new basis (3-332d), both the reps $\mathcal{D}(H)$ and $\mathcal{D}(G)$ become block–diagonal, that is,

$$\mathcal{D}(G) \to \sum_{\nu} \oplus \tau_\nu D^{(\nu)}(G) \ , \tag{3-333a}$$

where

$$D^{(\nu)}_{m'm}(R) = \langle \psi^{(\nu)\kappa}_{m'} | R | \psi^{(\nu)\kappa}_{m} \rangle \ . \tag{3-333b}$$

According to Schur's Lemma (3-319b),

$$\mathcal{D}(H) \to \sum_{\nu} \oplus h_\nu D^{(\nu)}(H) \ , \tag{3-334a}$$

$$D^{(\nu)}_{\kappa'\kappa}(H) = \langle \psi^{(\nu)\kappa'}_{m} | H | \psi^{(\nu)\kappa}_{m} \rangle \ . \tag{3-334b}$$

It is interesting to note that (a) the eigenspace of $(C, C(s)), \mathcal{L}_{(\nu)m} = \{\psi^{(\nu)\kappa}_m : \kappa = 1, 2, \ldots, \tau_\nu\}$ is an invariant subspace for both the Hamiltonian H and the intrinsic operator set $\overline{C}(s')$ introduced in (3-260). However, H does not commute with $\overline{C}(s')$ which is a CSCO of the subspace $\mathcal{L}_{(\nu)m}$, otherwise H would be a function of $\overline{C}(s')$; (b) the dimension of the matrix $D^{(\nu)}(H)[D^{(\nu)}(G)]$ is equal to the number of times that the matrix $D^{(\nu)}(G)[D^{(\nu)}(H)]$ occurs in the rep $\mathcal{D}(G)$, $[\mathcal{D}(H)]$. Therefore, the eigenequation (3-332c) is decomposed into N expectation equations with the much lower orders τ_ν,

$$\det | D^{(\nu)}(H) - E\, I |_1^{\tau_\nu} = 0 \ . \tag{3-334c}$$

In general, τ_ν is much smaller than n. In this way, the problem of solving the Schrödinger equation is greatly simplified.

Suppose that in (3-334c) there are n_ν distinct eigenvalues E^ν_i, $i = 1, 2, \ldots, n_\nu$, each with the degeneracy θ^ν_i. For a given E^ν_i, from (3-334c) we can get θ^ν_i eigenfunctions of the Hamiltonian,

$$\begin{gathered} \Psi^{(\nu)\theta}_m(E^\nu_i) = \sum_{\kappa=1}^{\tau_\nu} a^\theta_\kappa(E^\nu_i) \psi^{(\nu)\kappa}_m \ , \quad \tau_\nu = \sum_{i=1}^{n_\nu} \theta^\nu_i \ , \\ i = 1, 2, \ldots, n_\nu, \quad \theta = 1, 2, \ldots, \theta^\nu_i \ . \end{gathered} \tag{3-335}$$

Note that the degeneracy of the energy level E^ν_i is $\theta^\nu_i h_\nu$.

If in (3-334c) there are τ_ν distinct eigenvalues, $E^\nu_i, i = 1, 2, \ldots, \tau_\nu$, then E^ν_i can serve as the multiplicity label κ in (3-332d) for differentiating the τ_ν sets of equivalent bases of the irrep ν. In this case, the degeneracy of the energy E^ν_i is equal to the dimension of the irrep ν, and $\big(H, C, C(s)\big)$ provides a complete set of labels as discussed in Sec. 3.18.2.

If a certain irrep ν occurs only once in the rep $\mathcal{D}(G)$, i.e., $\tau_\nu = 1$, then the irreducible basis $\psi^{(\nu)}_m$ is just the eigenfunction of the Hamiltonian, $\Psi^{(\nu)}_m(E) = \psi^{(\nu)}_m$. This means that for this special case we can obtain the eigenfunction of the Hamiltonian from group theory alone. Of course, this happens only for very special energy levels; otherwise quantum mechanics could be replaced by group theory and this is evidently absurd.

3. *Two kinds of degeneracy.*

According to Theorem 2.7, the degenerate wave functions belonging to the same energy E carry a rep $\mathcal{D}^E$ for the group G, which is in general reducible.

Non-accidental degeneracy: If the rep $\mathcal{D}^E(G)$ is irreducible, say it is the irrep $D^{(\nu)}$, then the degeneracy of the energy level E is equal to the dimension h_ν of the irrep ν, and the eigenvalue of the operator $C(s)$ provides enough labels to distinguish the degenerate states with the energy E. This kind of degeneracy is called *non-accidental degeneracy* since it is entirely due to the inherent symmetry of the system, and it can not be reduced without lowering the symmetry of the system.

Accidental degeneracy: If the rep $\mathcal{D}^E(G)$ is reducible, $\mathcal{D}^E = \sum_\nu \theta_\nu D^{(\nu)}$, the degeneracy of the energy level is equal to $\sum_\nu \theta_\nu h_\nu$. Sometimes it is called accidental degeneracy. However,

one should distinguish the following two cases. (a) The full degeneracy may happen by chance or by design. For example, a numerical parameter in the Hamiltonian may be adjusted until two energy levels cross. This is truly an *accidental degeneracy.* (b) If, however, one finds what appear to be systematic accidental degeneracies, not just a single level, but in many levels, then it is usually a sign that the degeneracies are not accidental, but are due to the existence of some hitherto unsuspected higher symmetry. In such cases, one should not use the word "accidental."

As an example, consider the hydrogen atom for which the potential is $V = -1/r$. The obvious symmetry group is the rotation group R_3. The energy of the hydrogen atom depends only on the principal quantum number n but is independent of the angular momentum l, which is the irrep label for R_3 (Sec. 6.3). Therefore, the rep $\mathcal{D}^{(n)}$ of R_3 carried by the degenerate wave functions with the same energy E_n is reducible: $\mathcal{D}^{(n)} = \sum_{l=0}^{n} \oplus D^{(l)}$. These degeneracies are systematic and are due to the fact that the hydrogen has a higher symmetry group, the four-dimensional rotation group R_4 (Wybourne 1974). The generators of the group R_4 are the three components of the angular momentum, L_x, L_y, and L_z, and the three components of the vector

$$\mathbf{A} = -\left[\frac{1}{2Me^2}(\mathbf{p}\times\mathbf{L} - \mathbf{L}\times\mathbf{p}) - \frac{\mathbf{r}}{r}\right] .$$

For the alkali atom, $V = -1/r + \varepsilon/r^2$, the degeneracy of the energy in l is lifted, but the degeneracies in the magnetic quantum number m persist. The $(2l+1)$-fold degeneracy is non-accidental which is characteristic of the central force and cannot be reduced without breaking the rotational symmetry of the potential.

3.20.2. Splitting of the energy level due to a perturbation

Let $H = H_0 + H_1$, where H_0 is the principle term and H_1 is a perturbation. We also assume that

$$[H_0, G] = 0, \quad [H_1, G_1] = 0, \quad \text{but } [H_1, G] \neq 0 , \tag{3-336}$$

where G_1 is a subgroup of G. After the onset of the perturbation, the symmetry group of the system is lowered from G to G_1.

Evidently, the best way to treat such a system is to use the $G \supset G_1 \supset G_1(s)$ irreducible basis $\psi^{(\nu)}_{\Lambda m}$, where for simplicity we assume that $G \supset G_1 \supset G_1(s)$ is a canonical subgroup chain, and $G_1(s)$ can be chosen arbitrarily so long as $G_1 \supset G_1(s)$ is canonical. According to (3-320) we have

$$\langle \psi^{(\nu)}_{\Lambda m} | H_0 | \psi^{(\nu')}_{\Lambda' m'} \rangle = E^{(0)}_{\nu} \delta_{\nu\nu'} \delta_{\Lambda\Lambda'} \delta_{mm'} , \tag{3-337a}$$

$$\langle \psi^{(\nu)}_{\Lambda m} | H_1 | \psi^{(\nu')}_{\Lambda' m'} \rangle = E^{(1)}_{\nu\nu'\Lambda} \delta_{\Lambda\Lambda'} \delta_{mm'} . \tag{3-337b}$$

The diagonal element of H_1 is

$$\langle \psi^{(\nu)}_{\Lambda m} | H_1 | \psi^{(\nu)}_{\Lambda m} \rangle = E^{(1)}_{\nu\Lambda} . \tag{3-337c}$$

Without the perturbation, the symmetry group of the system is G, and ν, Λ, and m are all good quantum numbers, and the degeneracy of each energy level, if there is no accidental degeneracy, is h_ν.

With the perturbation, only Λ and m are good quantum numbers, while ν is only an approximate quantum number, and each level $E^{(0)}_{\nu}$ is split into several sub levels, as schematically shown in Fig. 3.20. The number of the sub levels is determined by the subduction of the irrep $D^{(\nu)}$ of G with respect to its subgroup G_1.

$$D^{(\nu)} \downarrow G_1 = \sum_{\Lambda} \oplus \tau_\Lambda D^{(\Lambda)}, \tag{3-337d}$$

where the multiplicity τ_Λ can be decided upon from (3-249b). The magnitude of the splitting is determined by (3-337c). Assuming that there is no accidental degeneracy, the degeneracy of each sub level Λ is equal to the dimension h_Λ of the irrep Λ of G_1.

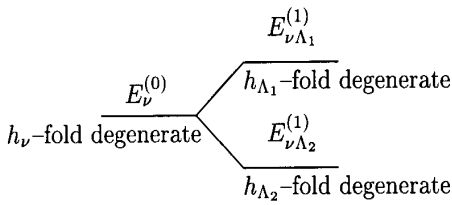


Fig. 3.20. The splitting of energy levels due to symmetry breaking.

We thus see that with the help of group theory, we can easily predict the number of the sub levels into which a given original energy level is split, as well as the magnitude of the splitting. Furthermore, the $G \supset G_1 \supset G_1(s)$ irreducible basis is the approximate (without considering the mixing of the various irreps of G) wave function for the perturbed Hamiltonian.

3.20.3. Dynamical symmetry

If the Hamiltonian of a system is a function of the CSCO of the subgroups contained in a group chain $G \supset G_1 \supset G_2 \supset \ldots$, we say that the system has a dynamical symmetry. Letting C_i be the CSCO of G_i, we have

$$H = F(C, C_1, C_2, \ldots) = F(C, C(s)) \ , \tag{3-338a}$$

where $C(s) = (C_1, C_2, \ldots)$. In this case, $[H, G] \neq 0$; however

$$[H, C] = 0, \quad [H, C(s)] = 0 \ . \tag{3-338b}$$

Therefore the eigenvalues (ν, m) of $(C, C(s))$ are good quantum numbers. Naturally, we choose the $G \supset G_1 \supset G_2 \supset \ldots$ irreducible basis as our basis for the system. In this basis, the Hamiltonian is diagonalized. Thus we can obtain an analytic expression for the energy

$$E = F(\nu, \mu_1, \mu_2, \ldots) = F(\nu, m) \ , \tag{3-338c}$$

without having to solve the Schrödinger equation.

The dynamical symmetry induces splitting of the energy level associated with an irrep of G, but not mixing of the energy levels associated with different irreps of G. There are many examples of dynamical symmetries. Sections 9.5–9.10 are devoted to the various dynamical symmetries of nuclei.

3.20.4. The general case

For the general case which does not fall into the previous three cases, group theory still plays an important role in the many-body problem. We may choose an appropriate group chain $G \supset G(s)$ and use the $G \supset G(s)$ irreducible basis to diagonalize the Hamiltonian. The appropriate group chain means that (1) $G(s)$ contains the symmetry group of the system and (2) the matrix elements of the Hamiltonian H in the basis are easily calculable (see Chap. 9).

3.20.5. Selection rules

Suppose that the operators inducing transitions between energy levels form an irreducible tensor of the symmetry group G of a system. According to the Wigner–Eckart theorem (3-317), the transition amplitude between two states belonging to the irreps ν_i and ν_f is proportional to

$$\langle \psi^{(\nu_f)}_{m_f} | T^{(\nu)}_m | \psi^{(\nu_i)}_{m_i} \rangle = \sum_\tau \left(C^{(\nu_f)\tau, m_f}_{\nu_i m_i, \nu m} \right)^* \langle \psi^{(\nu_f)} \| T^{(\nu)} \| \psi^{(\nu_i)} \rangle^{(\tau)} \ . \tag{3-339}$$

If the irrep ν_f is not contained in the Kronecker product $(\nu) \times (\nu_i)$, then the CG coefficient in (3-339) is zero, and the transition amplitude vanishes. Therefore, based on the CG series of the

symmetry group G, we can predict which transitions are forbidden. For the simply reducible case, (3-339) also gives the relative strengths of transitions from a given initial state $\psi_{m_i}^{(\nu_i)}$ to different final states belonging to the same irrep ν_f,

$$|\langle\psi_{m_f'}^{(\nu_f)}|T_{m'}^{(\nu)}|\psi_{m_i}^{(\nu_i)}\rangle|^2 \Big/ |\langle\psi_{m_f}^{(\nu_f)}|T_{m}^{(\nu)}|\psi_{m_i}^{(\nu_i)}\rangle|^2 = \left(C_{\nu_i m_i,\nu m'}^{\nu_f,m_f'}\right)^2 \Big/ \left(C_{\nu_i m_i,\nu m}^{\nu_f,m_f}\right)^2 .$$

Hence from the CG coefficients we can infer the relative strengths of the transitions.

Ex. 3.21. Show that in the Kronecker product space the projection operator is equal to $P_{mk}^{(\nu)} = \sum_{\tau=1}^{(\nu_1\nu_2\nu)} |\nu m\tau\rangle\langle\nu k\tau|$.

Ex. 3.22. Using Theorem 2.2, $[C, \overline{C}(s)] = 0$, as well as the property of C that it is a CSCO of the class space, is it possible to conclude that the intrinsic operator set $\overline{C}(s)$ is a function of C?

3.21. Summary

Thus far, all the important theorems for finite groups have been re-established through a route quite different from the traditional one. The traditional approach relies heavily on the character theory, whereas the new approach is based on the decomposition of the regular rep space by a set of commuting operators. The former approach may seem to be more elegant from a mathematical point of view. However, it has the serious drawback that it does not provide us with any practical method for reducing the regular rep. The new approach, though a bit lengthy in proving some theorems, is very instructive in nature. It not only offers more insights into the group structure, thereby revealing the duality between the group G and its intrinsic group $\overline{G}$, but also gives a simple and universal method for decomposing the regular rep into irreps subduced according to any given subgroup chain without knowledge of the characters. Consequently, the main advantages of the new approach are its applicability and flexibility.

The basic contents of this chapter can be summarized in the following seven theorems.

Theorem I: The eigenoperator $P^{(\nu)}$ of the CSCO–I of G in the class space is the projection operator onto the irrep (ν) of G,

$$\begin{aligned} CP^{(\nu)} &= \nu P^{(\nu)}, \\ P^{(\nu)} &= \frac{h_\nu}{g} \sum_i \left(\chi_i^{(\nu)}\right)^* C_i . \end{aligned} \tag{3-340}$$

Theorem II: The eigenfunctions of the CSCO–I of G in the space of functions on classes are complex conjugates of the simple characters

$$C\chi^{(\nu)}(C_i)^* = \nu\chi^{(\nu)}(C_i)^* . \tag{3-341}$$

The eigenfunctions of the CSCO–I obey the orthonormality and completeness relations

$$\sum_{i=1}^{N} \frac{g_i}{g} \chi^{(\nu)}(C_i)^* \chi^{(\nu')}(C_i) = \delta_{\nu\nu'} , \tag{3-342}$$

$$\sum_{\nu=1}^{N} \frac{g_i}{g} \chi^{(\nu)}(C_i)^* \chi^{(\nu)}(C_j) = \delta_{ij} . \tag{3-343}$$

The simple characters can be determined from (3-341) and (3-342).

Theorem III: A necessary and sufficient condition for $\psi^{(\nu)}$ to belong to the irrep (ν) of G is that $\psi^{(\nu)}$ satisfies the eigenequation

$$C\psi^{(\nu)} = \nu\psi^{(\nu)} . \tag{3-344}$$

Theorem IV: A necessary and sufficient condition for $\psi_m^{(\nu)}$ to belong to the irreps (ν, m) of the group chain $G \supset G(s)$ is that $\psi_m^{(\nu)}$ satisfy the eigenequations

$$\begin{pmatrix} C \\ C(s) \end{pmatrix} \psi_m^{(\nu)} = \begin{pmatrix} \nu \\ m \end{pmatrix} \psi_m^{(\nu)} . \tag{3-345}$$

If $G \supset G(s)$ is a canonical subgroup chain, then $(C, C(s))$ is a CSCO–II of G.

Theorem V: A necessary and sufficient condition for $\psi_m^{(\nu)\kappa}$ to belong to the irreps (ν, m) and (ν, κ) of the group chains $G \supset G(s)$ and $\overline{G} \supset \overline{G}(s')$, respectively, is that $\psi_m^{(\nu)\kappa}$ satisfy the eigenequations

$$\begin{pmatrix} C \\ C(s) \\ \overline{C}(s') \end{pmatrix} \psi_m^{(\nu)\kappa} = \begin{pmatrix} \nu \\ m \\ \kappa \end{pmatrix} \psi_m^{(\nu)\kappa} . \tag{3-346}$$

Here the intrinsic subgroup chain $\overline{G}(s')$ does not necessarily correspond to the subgroup chain $G(s)$. If $G \supset G(s)$ is a canonical subgroup chain, then $(C, C(s), \overline{C}(s))$ is a CSCO–III of G.

Theorem VI: The eigenoperator of the CSCO–III of G in the group space is the projection operator $P_{m\kappa}^{(\nu)}$

$$\begin{pmatrix} C \\ C(s) \\ \overline{C}(s) \end{pmatrix} P_{mk}^{(\nu)} = \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} P_{mk}^{(\nu)} . \tag{3-347}$$

$$P_{mk}^{(\nu)} = \frac{h_\nu}{g} \sum_a D_{mk}^{(\nu)*}(R_a) R_a . \tag{3-348}$$

Theorem VII: The eigenfunctions of the CSCO–III of G in the space of functions on the group (manifold) are complex conjugates of the irreducible matrix elements in the $G \supset G(s)$ basis,

$$\begin{pmatrix} C \\ C(s) \\ \overline{C}(s) \end{pmatrix} D_{mk}^{(\nu)*}(R_a) = \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} D_{mk}^{(\nu)*}(R_a) . \tag{3-349}$$

The eigenfunctions of the CSCO–III of G satisfy the orthonormality and completeness

$$\sum_a \frac{h_\nu}{g} D_{mk}^{(\nu)*}(R_a) D_{m'k'}^{(\nu')}(R_a) = \delta_{\nu\nu'} \delta_{mm'} \delta_{kk'} , \tag{3-350a}$$

$$\sum_{\nu mk} \frac{h_\nu}{g} D_{mk}^{(\nu)*}(R_a) D_{mk}^{(\nu)}(R_b) = \delta_{ab} . \tag{3-350b}$$

From the Eqs. (3-349) and (3-350a) we can determine the irreducible matrix elements.

Chapter 4

Representation Theory of the Permutation Group

The permutation group has important applications to the physics of many–particle systems. The importance lies in that a system of identical particles has permutation symmetry, and that there exist many deep and delicate inter–relations between the permutation group and the unitary group. The rep theory of the permutation group is well established through the efforts of Young, Frobenius, Yamanouchi and others. This theory has many advantages. For example, it gives the branching law for reducing the irrep of S_n into those of S_{n-1}, and an intuitive and elegant way of labelling the irreps and the irreducible bases by the Young diagrams and the Young tableaux.

However, from the practical point of view, this theory has some serious shortcomings. (1) It is too difficult for physicists to grasp the theory quickly. Soklov(1956) pointed out: "Due to the fact that group theory, especially the theory of representations and characters of the permutation group, is extremely difficult even for the specialists, there arose the tendency of opposing the so–called 'group-pest' in quantum mechanics." (2) When it comes to actual calculation, it is rather tedious to obtain the characters, the Yamanouchi bases, the Clebsch–Gordan coefficients, and so on.

From the general theory for finite groups and the example of the permutation group S_3 in the last chapter, it is seen that the new approach to group rep theory is an independent theory in the sense that we can obtain, through straightforward, standard and easily programmable methods, all the results without using the traditional Young–Yamanouchi theory. Nevertheless, it has its own drawbacks, namely, it is not possible to obtain general conclusions about the dimensionality of irreps and the branching law prior to concrete calculations.

From the above discussion it is seen that the advantages and disadvantages of the Young–Yamanouchi theory and the new approach to the permutation group are complementary. One's advantage is the other's disadvantage. Thus, from the practical point of view, we can combine these two to give a powerful method for handling the rep of the permutation group.

The first four sections of this chapter deal mainly with the relations between the new and old theories of the permutation group and some general conclusions obtained using the traditional theory of the permutation group. They are simple in themselves, yet the paths along which these conclusions were reached are by no means straightforward. Readers interested in the traditional theory of permutation groups and the origins of such conclusions are referred to Rutherford (1948) and Hamermesh (1962). The remaining sections of this chapter deal with the problem of how to use these general conclusions borrowed from the traditional theory of the permutation group to simplify the calculation based on the EFM.

4.1. Partitions, Young Diagrams and Eigenvalues of CSCO–I

In the traditional theory of the permutation group, we use partitions or the Young diagrams to label the irreps of the permutation group S_n.

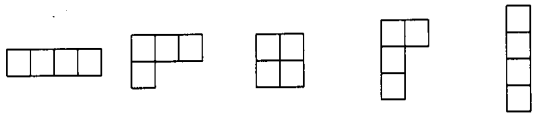
A *partition* is the splitting–up of n into an ordered list of n integers ν_i satisfying

$$\begin{aligned} n &= \nu_1 + \nu_2 + \ldots + \nu_n \ , \\ \nu_1 &\geq \nu_2 \geq \ldots \geq \nu_n \geq 0 \ . \end{aligned} \tag{4-1}$$

For example, 4=4+0+0+0, 4=3+1+0+0, 4=2+2+0+0, 4=2+1+1+0 and 4=1+1+1+1 are the only partitions of 4. We designate partitions by the symbol $[\nu] = [\nu_1\nu_2\ldots\nu_n]$. We usually drop those ν_i's which are zeroes. Thus $n = 4$ has the following partitions [4], [31], [22], [211], and [1111], or in abbreviated form [4], [31], [2^2], [21^2] and [1^4]. In the traditional theory of the permutation group irreps of the group S_n are labelled by partitions of n. The number of partitions of n is just the number of inequivalent irreps of S_n.

A partition $[\nu_1\nu_2\ldots]$ can be pictured as a *Young diagram* in which boxes are arranged in rows and columns with ν_i boxes occupying the first ν_i positions (counted from the left) of the i–th row. As an example, the Young diagrams corresponding to the partitions of $n = 4$ are

[4] [31] [22] [211] [1^4]



(4-2)

There is a one–to–one correspondence between the eigenvalues of the CSCO–I of S_n and the partitions or Young diagrams. It can be proved (see Eqs. (4-25) and (7-38d)) that the relations between the eigenvalues of the 2–cycle and 3–cycle class operators and the partitions $[\nu] = [\nu_1\nu_2\ldots\nu_k]$ are given by

$$\begin{aligned} \lambda^{(\nu)}_{(2)} &= \frac{n}{2} + \frac{1}{2}\sum_{l=1}^{k} \nu_l(\nu_l - 2l) \ , \\ \lambda^{(\nu)}_{(3)} &= \frac{1}{3}\left\{ 2n - \frac{3}{2}n^2 + \sum_{l=1}^{k} \nu_l\left[\nu_l^2 - \left(3l - \frac{3}{2}\right)\nu_l + 3l(l-1)\right]\right\}. \end{aligned} \tag{4-3}$$

In Table 3.2-1 the eigenvalues $\lambda^{(\nu)}_{(2)}$ and $\lambda^{(\nu)}_{(3)}$ are listed along with the corresponding partitions.

Using the conclusion that each partition uniquely labels an irrep of the permutation group and the relation (4-3) or the like (such as the relation between the eigenvalues of 4–cycle class operator and the partitions), we can easily find the CSCO–I of the permutation group. For example, if $\lambda^{(\nu)}_{(2)}$ are distinct for all partitions of n, then the 2–cycle class operator $C_{(2)}$ is a CSCO–I of S_n. Otherwise, we look at the pairs of values $(\lambda^{(\nu)}_{(2)}, \lambda^{(\nu)}_{(3)})$; if they are different for all partitions of n, then $(C_{(2)}, C_{(3)})$ is a CSCO–I of S_n, and so on.

An irrep of S_n can be labelled by a partition of n because a partition $[\nu] = [\nu_1, \nu_2, \ldots \nu_n]$ corresponds to a class label $(\nu) = (\nu_1\nu_2\ldots\nu_n)$ of S_n, and the number of inequivalent irreps of S_n is equal to the number of classes.

Two Young diagrams or partitions are said to be *conjugate* if they are obtained from each other by an interchange of rows and columns. The partition conjugate to $[\nu]$ is designated as $[\tilde{\nu}]$. For example, in (4-2), [31] and [211] are conjugate partitions. A Young diagram $[\nu]$ is said to be *self–conjugate* if $[\nu] = [\tilde{\nu}]$. For example, [22] and [311] are self–conjugate. Two reps labelled by $[\nu]$ and $[\tilde{\nu}]$ are called *conjugate reps* (not to be confused with the complex conjugate rep). A rep labelled by self–conjugate Young diagram is called a *self–conjugate rep.* It is clear that conjugate reps always appear in pairs.

4.2. Characters of Permutation Groups

The Frobenius theory of characters (Hamermesh 1962) plays a crucial role in the traditional theory of the permutation group. It is an elegant, but very difficult theory.

The *dimension of the irrep* $[\nu] = [\nu_1\nu_2\ldots\nu_k]$ of the permutation group S_n is given by the Frobenius formula (Bohr 1969)

$$h_{[\nu]} = \chi_e^{(\nu)} = n! \prod_{i<j\leq k} (\nu_i - \nu_j + j - i) \Big/ \prod_{i=1}^{k} (\nu_i + k - i)! \,. \tag{4-4a}$$

A simpler formula is given by Robinson (1961). With each box of a Young diagram we associate a *hook* consisting of the given box (the head node) together with all those boxes that are to the right in the same row and lower in the same column as the head node. The number of boxes in the hook is called the *hook length.* The dimension $h_{[\nu]}$ can be expressed as

$$h_{[\nu]} = n! \Big/ \prod_i l_i \,, \tag{4-4b}$$

where $\Pi_i l_i$ is the product of all the hook lengths in the Young diagram $[\nu]$. For example

$$h_{[31]} = \frac{4!}{\begin{array}{|c|c|c|c|}\hline 4 & 2 & 1 \\ \hline 1 \\ \cline{1-1}\end{array}} = \frac{4!}{4\times 2\times 1\times 1} = 3 \,,$$

$$h_{[321]} = \frac{6!}{\begin{array}{|c|c|c|c|}\hline 5 & 3 & 1 \\ \hline 3 & 1 \\ \cline{1-2} 1 \\ \cline{1-1}\end{array}} = \frac{6!}{5\times 3\times 3\times 1\times 1\times 1} = 16 \,.$$

The dimensions of the irreps of the permutation groups up to S_6 are given in Table A1 of the Appendix.

For the simple characters of the permutation groups up to S_7, see Hamermesh (1962) p. 276, up to S_{10}, see Littlewood (1958). The EFM can also be used to calculate the simple characters of the permutation group. The characters of S_{11} have been calculated in this way by Gao (1976).

Ex. 4.1. Use Eq. (4-4b) to calculate the dimensions of the irreps of S_3–S_6.

In the Frobenius theory, using the so–called "regular application of r dots method," the relation between characters of conjugate representations has been shown to be

$$\chi_i^{(\tilde{\nu})} = \delta_i \chi_i^{(\nu)} \,, \tag{4-5}$$

where δ_i is the parity of the i–th class. This can be proved much more easily using the EFM.

Suppose the CSCO–I of S_n is $C = (C_1, \ldots, C_l)$. From (3-28) we know that $q_j^{(\nu)}$ satisfy the following sets of eigenequations

$$\sum_{j=1}^{N} C_{ij}^k q_j^{(\nu)} = \lambda_i^{(\nu)} q_k^{(\nu)}, \quad i = 1, 2, \ldots l \,. \tag{4-6}$$

Since the permutation parities on both sides of $C_iC_j = \sum_k C_{ij}^k C_k$ must be equal, we have

$$C_{ij}^k = 0, \quad \text{for} \quad \delta_i\delta_j \neq \delta_k \,. \tag{4-7}$$

From (4-6) and (4-7)

$$\sum_{j=1}^{N} C_{ij}^k (\delta_j q_j^{(\nu)}) = (\delta_i \lambda_i^{(\nu)})(\delta_k q_k^{(\nu)}), \quad i = 1, 2, \ldots, l \,. \tag{4-8}$$

Therefore if $\lambda^{(\nu)} = (\lambda_1^{(\nu)}, \ldots, \lambda_l^{(\nu)})$ is an eigenvalue set of C, then

$$\lambda^{(\tilde{\nu})} = (\delta_1 \lambda_1^{(\nu)}, \ldots \delta_l \lambda_l^{(\nu)}) \tag{4-9a}$$

is necessarily an eigenvalue set of C, and the eigenvector of the irrep $(\tilde{\nu})$ is

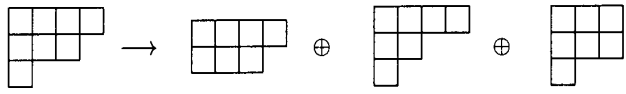
$$q_j^{(\tilde{\nu})} = \delta_j q_j^{(\nu)}, \quad j = 1, 2, \ldots, N \, . \tag{4-9b}$$

From this result and the relation $\chi_j^{(\nu)} = \sqrt{g} q_j^{(\nu)*}$ (Eq. (3-245)), we obtain (4-5).

4.3. Branching Laws, the Young–Yamanouchi Basis, and Young Tableaux

An irreducible representation $[\nu]$ of S_n is in general reducible with respect to its subgroup S_{n-1}, $[\nu] \downarrow S_{n-1} = \sum_{\nu'} \oplus D^{[\nu']}(S_{n-1})$, where the Young diagrams $[\nu']$ result from removing one box in all possible way in the Young diagram $[\nu]$, and each irrep $[\nu']$ occurs only once (Hamermesh 1962).

For example the irrep [431] of S_8 contains each of the irreps [43], [421] and [331] once.



Dimension: 70 = 14 + 35 + 21 (4-10)

In general, we have

$$[\nu_1 \nu_2 \ldots \nu_i \ldots \nu_n] = \sum_{i=n}^{1}{}' [\nu_1, \nu_2, \ldots \nu_i - 1, \ldots \nu_n]. \tag{4-11a}$$

The prime in the summation indicates the restrictions that we must have $\nu_i - 1 \geq 0$ and $\nu_i - 1 > \nu_{i+1}$ in order that $[\nu']$ is a Young diagram. The dimensions on both sides of (4-11a) must be equal; therefore

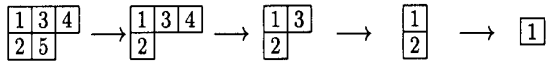
$$h_{[\nu_1 \ldots \nu_i \ldots \nu_n]} = \sum_{i=n}^{1}{}' h_{[\nu_1 \ldots \nu_i - 1 \ldots \nu_n]} \tag{4-11b}$$

Equation (4-11a) is referred to as the *branching law* for the permutation group.

The $S_n \supset S_{n-1} \supset \ldots \supset S_2 \supset S_1$ irreducible basis is now widely accepted as the *standard basis* of the permutation group. It is also called the *Young–Yamanouchi basis* . From the branching law (4-11a) and the fact that the group S_2 is Abelian, we know that the group chain $S_n \supset S_{n-1} \supset \ldots \supset S_2$ is canonical (the last group S_1 is redundant).

A *Young tableau* is an arrangement of the numbers 1,2...,n in a Young diagram in which numbers increase as one moves to the right and as one goes down. A Young tableau is denoted by $Y_m^{(\nu)}$, where m is the index of the tableau.

From a given Young tableau $Y_m^{[\nu]}$, one obtains another Young tableau $Y_{m'}^{[\nu']}$ involving $n-1$ numbers by removing the box containing the number n; by removing the box with the number $n-1$ one obtains yet another Young tableau $Y_{m''}^{[\nu'']}$ and so on. We use $|[\nu]m\rangle$ or $|Y_m^{[\nu]}\rangle$ to denote a *Yamanouchi basis vector* . The symbol $|Y_m^{[\nu]}\rangle$ will stand for an irreducible basis vector belonging to the irrep $[\nu], [\nu'], [\nu''] \ldots, [1]$ of the group $S_n, S_{n-1}, S_{n-2}, \ldots, S_1$. For example



[32] [31] [21] [11] [1] (4-11c)

The irreducible basis vector $\begin{array}{|c|c|c|}\hline 1 & 3 & 4 \\ \hline 2 & 5 \\ \cline{1-2}\end{array}$ thus belongs to the irreps [32], [31], [21], [11] and [1] of the groups S_5, S_4, S_3, S_2 and S_1, respectively. The irrep of the last group S_1 is always [1], and thus can be omitted. The decomposition of a Young tableau is consistent with the branching law.

The labelling by the sequence $[\nu], [\nu'], [\nu''], \ldots, [1]$ is complete in the sense that no two basis vectors of S_n will have the same sequence and that, to every sequence, there corresponds a basis vector of S_n. From the completeness of this labelling system, it follows immediately that the dimension of the irrep $[\nu]$ is equal to the number of distinct tableaux obtainable from the Young diagram $[\nu]$.

We can use the *Yamanouchi symbols* $(r_n r_{n-1} \ldots r_2 r_1)$ to label a Yamanouchi basis vector, where r_i is the row number of the letter i in the Young tableau. According to the definition of the Young tableaux, the letter 1 is always in the upper left-hand corner of a Young tableau; therefore $r_1 \equiv 1$.

Once we have Yamanouchi symbols for each Young tableau of the irrep $[\nu]$, we arrange them in decreasing page order and assign an index m to each symbol. For example

Young tableaux	$\begin{array}{\|c\|c\|c\|}\hline 1&2&3\\\hline 4\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|c\|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|c\|}\hline 1&3&4\\\hline 2\\\cline{1-1}\end{array}$
Yamanouchi symbols	(2111)	(1211)	(1121)

The largest Yamanouchi symbol corresponds to the smallest index $m = 1$. The Young tableaux for permutation groups up to S_6 are listed in Table 4.4-1. The Yamanouchi symbols for S_3–S_5 are listed in Table 4.4-2. For typographical reasons, we often delete the square boxes in Young tableaux in the following.

4.4. Yamanouchi Matrix Elements

From the branching law (4-11a) and since the Yamanouchi basis is an irreducible basis classified according to the irreps of $S_n \supset S_{n-1} \supset \ldots \supset S_2$, we know that in the irrep $[\nu]$ of S_n, the representatives $D^{[\nu]}(R)$ of the elements R belonging to the subgroup S_{n-1} must take the block-diagonal form

$$D^{[\nu_1 \ldots \nu_i \ldots \nu_n]}(R) = \sum_{i=n}^{1} \oplus D^{[\nu_1 \ldots \nu_i - 1 \ldots \nu_n]}(R), \quad R \in S_{n-1} \,. \tag{4-12}$$

For example, corresponding to Eq. (4-10) we have

$$D^{[431]}(R) = \begin{pmatrix} D^{[43]}(R) & & \\ & D^{[421]}(R) & \\ & & D^{[331]}(R) \end{pmatrix}, \quad R \in S_7 \,. \tag{4-13}$$

More examples can be found in Table 4.4-2.

Once one knows the irreducible matrices of the $n-1$ generators of S_n, (12), (23),..., $(n-1, n)$ the irreducible matrices of all elements of S_n can be found from (1-8a), (1-9) and the like.

There is a simple rule for finding the irreducible matrix elements of the adjacent transpositions $(i, i-1), i = 2, 3, \ldots, n$ in the Yamanouchi basis of S_n:

1. The basis vector $|Y_m^{[\nu]}\rangle$ is symmetric (antisymmetric) in $i-1$ and i if they are in the same row (column) of the Young tableau $Y_m^{[\nu]}$,

$$(i-1, i)|Y_m^{[\nu]}\rangle = \pm |Y_m^{[\nu]}\rangle \tag{4-14a}$$

2. If $i-1$ and i are neither in the same row nor the same column of $Y_m^{[\nu]}$,

$$\begin{aligned} D^{[\nu]}_{m'm}(i-1, i) &= \langle Y_{m'}^{[\nu]} | (i-1, i) | Y_m^{[\nu]} \rangle \cdot \\ &= \begin{cases} 1/\sigma \,, & m' = m \\ \sqrt{\sigma^2 - 1}/|\sigma| \,, & \text{when } Y_{m'}^{[\nu]} = (i-1, i) Y_m^{[\nu]} \,, \\ 0 & \text{otherwise} \,, \end{cases} \end{aligned} \tag{4-14b}$$

Table 4.4-1. The phase factors $\Lambda_m^{[\nu]}$*, Young tableaux $Y_m^{[\nu]}$ and the corresponding eigenvalues $\lambda=\Sigma_{f=3}^{n}(2f-5)\lambda_f$.**

$[\nu]$	[21]		[31]			[22]		[211]		
m	1	2	1	2	3	1	2	1	2	3
Λ_m^ν	+	−	+	−	+	+	−	+	−	+
Y_ν^m	12 3	13 2	123 4	124 3	134 2	12 34	13 24	12 3 4	13 2 4	14 2 3
λ			9	6		0		-6		

$[\nu]$	[41]				[32]					[311]					
m	1	2	3	4	1	2	3	4	5	1	2	3	4	5	6
Λ_m^ν	+	−	+	−	+	−	+	+	−	+	−	+	+	−	+
Y_ν^m	1234 5	1235 4	1245 3	1345 2	123 45	124 35	134 25	125 34	135 24	123 4 5	124 3 5	134 2 5	125 3 4	135 2 4	145 2 3
λ	46	34	31		19	16		10		9	6		-6		

$[\nu]$	[221]					[2111]				[51]				
m	1	2	3	4	5	1	2	3	4	1	2	3	4	5
Λ_m^ν	+	−	−	+	−	+	−	+	−	+	−	+	−	+
Y_ν^m	12 34 5	13 24 5	12 35 4	13 25 4	14 25 3	12 3 4 5	13 2 4 5	14 2 3 5	15 2 3 4	12345 6	12346 5	12356 4	12456 3	13456 2
λ	-10		-16			-31				134	109	97	94	

$[\nu]$	[42]									[411]				
m	1	2	3	4	5	6	7	8	9	1	2	3	4	5
Λ_m^ν	+	−	+	−	+	−	+	+	−	+	−	+	−	+
Y_ν^m	1234 56	1235 46	1245 36	1345 26	1236 45	1246 35	1346 25	1256 34	1356 24	1234 5 6	1235 4 6	1245 3 6	1345 2 6	1236 4 5
λ	81	69	66		54	51		45		67	55	52		30

$[\nu]$	[411]					[33]					[321]			
m	6	7	8	9	10	1	2	3	4	5	1	2	3	4
Λ_m^ν	−	+	+	−	+	+	−	+	+	−	+	−	+	+
Y_ν^m	1246 3 5	1346 2 5	1256 3 4	1356 2 4	1456 2 3	123 456	124 356	134 256	125 346	135 246	123 45 6	124 35 6	134 25 6	125 34 6
λ			15			40	37		31		19	16		10

*The definition of $\Lambda_m^{[\nu]}$ is given in Sec. 4.7.

**See Eq. (4-31). The eigenvalues for the totally symmetric bases are

[3],	[4],	[5],	[6]
3	21	76	176

.

cont'd

$[\nu]$	[321]												[222]		
m	5	6	7	8	9	10	11	12	13	14	15	16	1	2	3
Λ^{ν}_{m}	−	−	+	−	−	+	−	−	+	+	−	+	+	−	−
Y^{m}_{ν}	135	123	124	134	125	135	145	126	136	126	136	146	12	13	12
	24	46	36	26	36	26	26	34	24	35	25	25	34	24	35
	6	5	5	5	4	4	3	5	5	4	4	3	56	56	46
λ		9	6		-6			-10		-16			-31		-37

$[\nu]$	[222]		$[31^3]$										[2211]		
m	4	5	1	2	3	4	5	6	7	8	9	10	1	2	3
Λ^{ν}_{m}	+	−	+	−	+	+	−	+	−	+	−	+	+	−	−
Y^{m}_{ν}	13	14	123	124	134	125	135	145	126	136	146	156	12	13	12
	25	25	4	3	2	3	2	2	3	2	2	2	34	24	35
	46	36	5	5	5	4	4	3	4	4	3	3	5	5	4
λ			-12	-15		-27			-52				-45		-51

$[\nu]$	[2211]						$[21^4]$				
m	4	5	6	7	8	9	1	2	3	4	5
Λ^{ν}_{m}	+	−	+	−	+	−	+	−	+	−	+
Y^{m}_{ν}	13	14	12	13	14	15	12	13	14	15	16
	25	25	36	26	26	26	3	2	2	2	2
	4	3	4	4	3	3	4	4	3	3	3
	6	6	5	5	5	4	5	5	5	4	4
							6	6	6	6	5
λ			-66				-94				

where σ is called the *axial distance* from $i-1$ to i in the Young tableau $Y^{[\nu]}_{m}$. It is defined as following: Starting from the position of $i-1$ in $Y^{[\nu]}_{m}$, we proceed by any rectangular route, one box at a time, until we reach the position of i. Counting plus one for each step made upwards or to the right, and minus one for each step made downwards or to the left, the resulting number of steps made will be the axial distance.

For $\begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3&5\\\cline{1-2}\end{array}$ and $\begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4&5\\\cline{1-2}\end{array}$ the axial distances from 3 to 4 are $+3$ and -3 respectively.

Thus

$$\left\langle \begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3&5\\\cline{1-2}\end{array} \right| (34) \left| \begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3&5\\\cline{1-2}\end{array} \right\rangle = +\tfrac{1}{3} \quad \left\langle \begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4&5\\\cline{1-2}\end{array} \right| (34) \left| \begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4&5\\\cline{1-2}\end{array} \right\rangle = -\tfrac{1}{3}$$

$$\left\langle \begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3&5\\\cline{1-2}\end{array} \right| (34) \left| \begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4&5\\\cline{1-2}\end{array} \right\rangle = \sqrt{\tfrac{8}{3}} \quad \left\langle \begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4&5\\\cline{1-2}\end{array} \right| (34) \left| \begin{array}{|c|c|c|}\hline 1&2&5\\\hline 3&4\\\cline{1-2}\end{array} \right\rangle = 0 \tag{4-15}$$

The *axial distance* can be calculated by

$$\sigma = c_i - c_{i-1} - (r_i - r_{i-1}), \tag{4-16}$$

where $r_i, r_{i-1}(c_i, c_{i-1})$ are the row (column) numbers of the letters i and $i-1$ in the Young tableau $Y^{[\nu]}_{m}$ respectively.

The standard method for deriving the Yamanouchi matrix elements (4-14b) is rather laborious. In Sec. 4.20, it will be derived easily using the EFM (Zhu 1983).

Care must be exercised to distinguish between the Young tableaux $Y_m^{[\nu]}$ and the basis vectors $|Y_m^{[\nu]}\rangle$. If $Y_{m'}^{[\nu]} = (i-1,i)Y_{m'}^{[\nu]}$ then according to Eq. (4-14b) we have

$$(i-1,i)|Y_m^{[\nu]}\rangle = \frac{1}{\sigma}\left|Y_m^{[\nu]}\right\rangle + \frac{\sqrt{\sigma^2-1}}{|\sigma|}\left|Y_{m'}^{[\nu]}\right\rangle \quad \text{and} \tag{4-17}$$

$$(i-1,i)|Y_m^{[\nu]}\rangle \neq |Y_{m'}^{[\nu]}\rangle = |(i-1,i)Y_m^{[\nu]}\rangle \ .$$

The off-diagonal matrix elements in Eq. (4-14b) are always chosen to be positive. This is called the *Yamanouchi phase convention*, and the matrix elements are called the *Yamanouchi matrix elements*. In this book we will also adopt this phase convention. Equation (4-14) hold for any $i = 2, \ldots, n$. Therefore a Yamanouchi basis vector $|Y_m^{[\nu]}\rangle$ is symmetric (anti-symmetric) with respect to any adjacent indices which are at the same row (column) in $Y_m^{[\nu]}$, but has no symmetry with respect to other indices (non-adjacent indices on the same row or column, or adjacent indices in different rows or columns). For example, the irreducible basis vector

$$\left|\begin{array}{|c|c|c|c|}\hline 1&2&3&11\\\hline 4&7&8\\\cline{1-3} 5&9&12\\\cline{1-3} 6&10\\\cline{1-2}\end{array}\right\rangle$$

is symmetric in the indices (1,2,3) and (7,8) and anti-symmetric in the indices (4,5,6) and (9,10), but has no definite symmetry with respect to other indices.

Ex. 4.2. Find the Yamanouchi matrices for the adjacent transpositions in [42] and [321].

Table 4.4-2 gives the Yamanouchi matrices of the adjacent permutations of S_3 to S_5. Since they are symmetric matrices, only the upper triangles of the matrices are given.

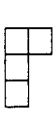
Table 4.4-2. Yamanouchi matrix elements of adjacent transpositions for $S_2 - S_5$.

S_3 : 

$$\begin{array}{c} \\ 211 \\ 121 \end{array} \quad \begin{array}{c} (12) \\ \begin{pmatrix} 1 & 0 \\ & -1 \end{pmatrix} \end{array} \quad \begin{array}{c} (23) \\ \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ & \frac{1}{2} \end{pmatrix} \end{array}$$

S_4 : 

$$\begin{array}{c} \\ 2111 \\ \\ 1211 \\ 1121 \end{array} \quad \begin{array}{c} (12) \\ \left(\begin{array}{c|cc} 1 & 0 & 0 \\ \hline & 1 & 0 \\ & & -1 \end{array}\right) \end{array} \quad \begin{array}{c} (23) \\ \left(\begin{array}{c|cc} 1 & 0 & 0 \\ \hline & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ & & \frac{1}{2} \end{array}\right) \end{array} \quad \begin{array}{c} (34) \\ \begin{pmatrix} -\frac{1}{3} & \frac{\sqrt{8}}{3} & 0 \\ & \frac{1}{3} & 0 \\ & & 1 \end{pmatrix} \end{array}$$

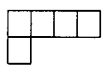


$$\begin{array}{c} \\ 3211 \\ 3121 \\ \\ 1321 \end{array} \quad \begin{array}{c} (12) \\ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ & -1 & 0 \\ \hline & & -1 \end{array}\right) \end{array} \quad \begin{array}{c} (23) \\ \left(\begin{array}{cc|c} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ & \frac{1}{2} & 0 \\ \hline & & -1 \end{array}\right) \end{array} \quad \begin{array}{c} (34) \\ \left(\begin{array}{ccc} -1 & 0 & 0 \\ & -\frac{1}{3} & \frac{\sqrt{8}}{3} \\ & & \frac{1}{3} \end{array}\right) \end{array}$$

$$\begin{array}{c} \\ 2211 \\ 2121 \end{array} \quad \begin{array}{c} (12) \\ \begin{pmatrix} 1 & 0 \\ & -1 \end{pmatrix} \end{array} \quad \begin{array}{c} (23) \\ \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ & \frac{1}{2} \end{pmatrix} \end{array} \quad \begin{array}{c} (34) \\ \begin{pmatrix} 1 & 0 \\ & -1 \end{pmatrix} \end{array}$$

cont'd

S_5 :



21111
12111
11211
11121

(12)

$$\left(\begin{array}{c|ccc} 1 & & & \\ \hline & 1 & 0 & 0 \\ & & 1 & 0 \\ & & & -1 \end{array}\right)$$

(23)

$$\left(\begin{array}{c|ccc} 1 & & & \\ \hline & 1 & 0 & 0 \\ & & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ & & & \frac{1}{2} \end{array}\right)$$

(34)

$$\left(\begin{array}{c|ccc} 1 & & & \\ \hline & -\frac{1}{3} & \frac{\sqrt{8}}{3} & 0 \\ & & \frac{1}{3} & 0 \\ & & & 1 \end{array}\right)$$

(45)

$$\left(\begin{array}{cccc} -\frac{1}{4} & \frac{\sqrt{15}}{4} & 0 & 0 \\ & \frac{1}{4} & 0 & 0 \\ & & 1 & 0 \\ & & & 1 \end{array}\right)$$

22111
21211
21121
12211
12121

(12)

$$\left(\begin{array}{ccc|cc} 1 & & & & \\ & 1 & & & \\ & & -1 & & \\ \hline & & & 1 & \\ & & & & -1 \end{array}\right)$$

(23)

$$\left(\begin{array}{ccc|cc} 1 & 0 & 0 & & \\ & -\frac{1}{2} & \frac{\sqrt{3}}{2} & & \\ & & \frac{1}{2} & & \\ \hline & & & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ & & & & \frac{1}{2} \end{array}\right)$$

(34)

$$\left(\begin{array}{ccc|cc} -\frac{1}{3} & \frac{\sqrt{8}}{3} & 0 & & \\ & \frac{1}{3} & 0 & & \\ & & 1 & & \\ \hline & & & 1 & 0 \\ & & & & -1 \end{array}\right)$$

(45)

$$\left(\begin{array}{ccccc} 1 & 0 & 0 & 0 & 0 \\ & -\frac{1}{2} & 0 & \frac{\sqrt{3}}{2} & 0 \\ & & -\frac{1}{2} & 0 & \frac{\sqrt{3}}{2} \\ & & & \frac{1}{2} & 0 \\ & & & & \frac{1}{2} \end{array}\right)$$

32111
31211
31121
13211
13121
11321

(12)

$$\left(\begin{array}{ccc|cc} 1 & & & & \\ & 1 & & & \\ & & -1 & & \\ \hline & & & 1 & \\ & & & & -1 \\ & & & & \end{array}\right)$$

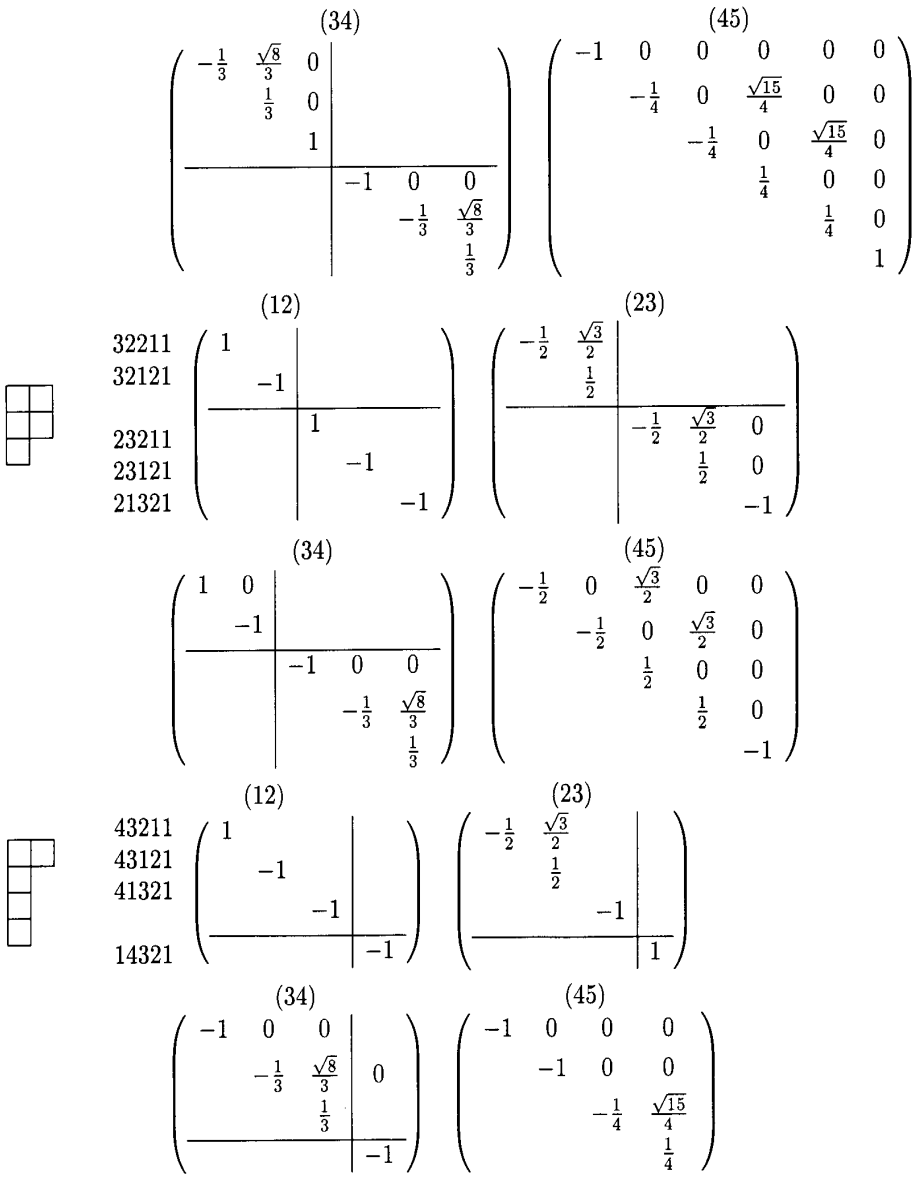
(23)

$$\left(\begin{array}{ccc|cc} 1 & 0 & 0 & & \\ & -\frac{1}{2} & \frac{\sqrt{3}}{2} & & \\ & & \frac{1}{2} & & \\ \hline & & & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ & & & & \frac{1}{2} \\ & & & & \end{array}\right)$$

$$\left(\begin{array}{ccc|c} & & & \\ & & & \\ & & & \\ \hline & & & 0 \\ & & & 0 \\ & & & -1 \end{array}\right)$$

The matrices (45), (15), (25), (35) for [32] on page 229 of Hamermesh (1962) are incorrect.

cont'd



4.5. The CSCO–II of Permutation Groups

Since the group chain $S_n \supset S_{n-1} \supset \ldots \supset S_2$ is canonical, the set of operators

$$M = (C(n),\ C(n-1), \ldots C(2)) \tag{4-18}$$

is a CSCO–II of S_n, where $C(f), f = n, \ldots 2$, is the CSCO–I of S_f. For $6 \leq f \leq 14, C(f)$ contains 2- and 3-cycle class operators $C_{(2)}(f)$, $C_{(3)}(f)$; for $f \geq 15, C(f)$ contains more operators. We are now going to prove that the set of operators $(C(n), \ldots, C(2))$ is over-complete.

Theorem 4.1: The $(n-1)$ 2-cycle class operators $(C_{(2)}(n), \ldots, C_{(2)}(2))$ of the group chain

$S_n \supset S_{n-1} \supset \ldots \supset S_2$ constitute a CSCO–II of S_n.

Proof: It suffices to prove that a Yamanouchi basis vector of S_n can be labelled uniquely by the eigenvalues $\lambda_n, \lambda_{n-1}, \ldots, \lambda_2$ of the $(n-1)$ 2–cycle class operators. For $n \leq 5$, a single class operator $C_{(2)}(n)$ is the CSCO–I of S_n, so the theorem is trivial for $n \leq 5$.

Now supposing it holds for S_n, we want to prove that it also holds for S_{n+1}. According to the branching law this in turn amounts to proving that if there are m Young diagrams $[\nu^1] \ldots [\nu^m]$ of S_{n+1}, which correspond to the same eigenvalue λ_{n+1}, and if $[\overline{\nu}^i]$ is a Young diagram resulting from removing one box from the Young diagram $[\nu^i]$ (see Fig. 4.5-1), then $[\overline{\nu}^i] \neq [\overline{\nu}^j]$ for $i \neq j$.

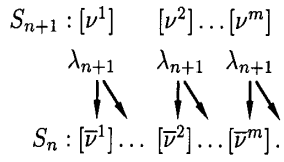


Fig. 4.5-1a. General branching.

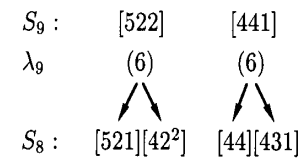


Fig. 4.5-1b. An example of branching.

It again amounts to proving that all the eigenvalues corresponding to the Young diagrams $[\mu^i]$ which result from adding one box to the same Young diagram $[\overline{\nu}]$ of S_n are distinct (see the Fig. 4.5-2). Let $[\mu^i]$ be the Young diagram resulting from adding one box in the i–th row of the Young diagram $[\overline{\nu}] = [\nu_1 \ldots \nu_i \ldots \nu_n]$,

$$[\mu^i] = [\nu_1, \nu_2, \ldots \nu_{i-1},\ \nu_i + 1,\ \nu_{i+1}, \ldots] \ , \tag{4-19}$$

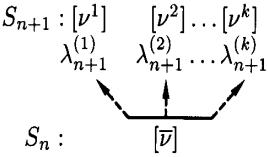


Fig. 4.5-2a. Inverse branching.

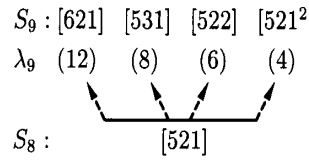


Fig. 4.5-2b. An example of inverse branching.

From Eq. (4-3a) and (4-19) one has

$$\lambda_{n+1}^{(i)} = (n+1)/2 + \frac{1}{2} \sum_l (\nu_l + \delta_{li})(\nu_l + \delta_{li} - 2l) \ . \tag{4-20}$$

If $\lambda_{n+1}^{(i)} = \lambda_{n+1}^{(j)}$, from Eq. (4-20) one has

$$\nu_i - i = \nu_j - j \ . \tag{4-21}$$

Supposing $i < j$, we must have $\nu_i \geq \nu_j$ because of the indexing rule for the Young diagrams. But then Eq. (4-21) holds only when $i = j$. The theorem is therefore proved. **QED**

Therefore the basis vectors of different irreps of S_n with the same eigenvalue λ_n must follow different routes in the process of reduction with respect to the subgroups $S_{n-1}, S_{n-2}, \ldots, S_2$. Consequently, even though the eigenvalues λ_n of the 2–cycle class operator $C_{(2)}(n)$ have degeneracies in the class space, the set of eigenvalues $(\lambda_n, \lambda_{n-1}, \ldots \lambda_2)$ can still label a Yamanouchi basis vector uniquely.

Henceforth, to simplify the notation, $C(n)$ is used to designate the 2–cycle class operator instead of $C_{(2)}(n)$, unless otherwise stated.

The above conclusion can be seen more clearly from the branching diagram. Figure 4.5-3 gives the branching law for S_n with $n \leq 6$. The numbers below each partition of S_n are the eigenvalues λ_n. Starting from each partition of S_n, each "flight route" along the arrows corresponds to a Yamanouchi basis vector of S_n. We can use either a sequence of partitions or a sequence of eigenvalues through which the route passes to label a basis vector.

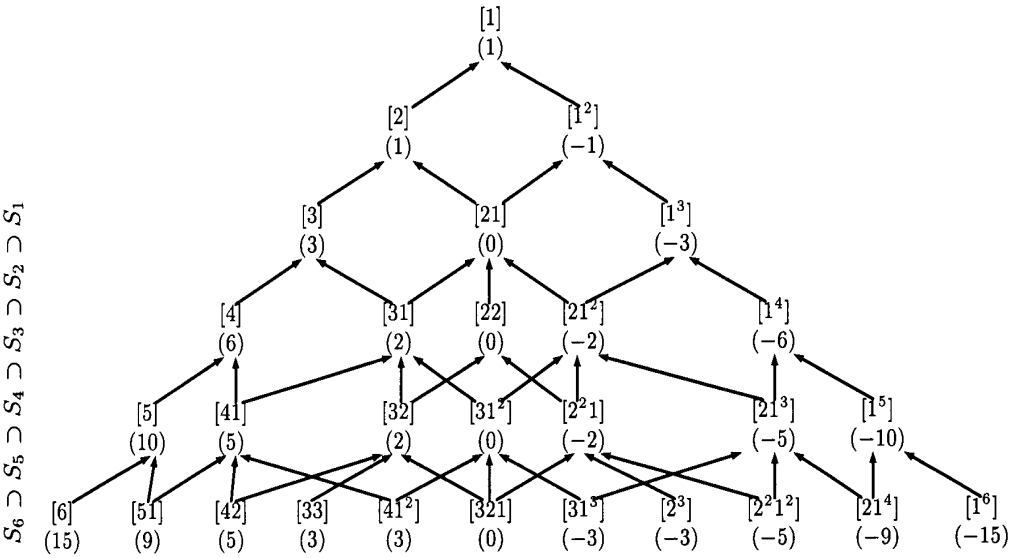


Fig. 4.5-3. The branching diagram for the group S_6.

Now we have three equivalent ways to *label* a Yamanouchi basis vector: the $(n-1)$ eigenvalues $(\lambda_n, \ldots, \lambda_2)$ of the CSCO-II of S_n, the Yamanouchi symbol $(r_n, \ldots, r_2, r_1 = 1)$, and the Young tableau. Any two are in a one–to–one correspondence. As an example, in Table 4.5 we list the three labelling schemes for bases of the irreps [411] and [33]. It is seen that the degeneracy of $\lambda_6 = 3$ does not prevent us from labelling the basis vectors uniquely by the set of eigenvalues $(\lambda_6, \lambda_5 \ldots, \lambda_2)$.

Table 4.5. Three kinds of labelling of the Yamanouchi basis for the irreps [411] and [33].

ψ_λ	$\psi_{3,5,6,3,1}$	$\psi_{3,5,2,3,1}$	$\psi_{3,5,2,0,1}$	$\psi_{3,5,2,0,-1}$	$\psi_{3,0,2,3,1}$
$\psi(r)$	$\psi(321111)$	$\psi(312111)$	$\psi(311211)$	$\psi(311121)$	$\psi(132111)$
Young tableau	1 2 3 4 5 6	1 2 3 5 4 6	1 2 4 5 3 6	1 3 4 5 2 6	1 2 3 6 4 5
ψ_λ	$\psi_{3,2,2,3,1}$	$\psi_{3,2,2,0,1}$	$\psi_{3,2,2,0,-1}$	$\psi_{3,2,0,0,1}$	$\psi_{3,2,0,0,-1}$
$\psi(r)$	$\psi(222111)$	$\psi(221211)$	$\psi(221121)$	$\psi(212211)$	$\psi(212121)$
Young tableau	1 2 3 4 5 6	1 2 4 3 5 6	1 3 4 2 5 6	1 2 5 3 4 6	1 3 5 2 4 6

The use of the eigenvalues to label a basis vector is easily acceptable to physicists. It has the

following special features:

1. The eigenvalues $\lambda_f, f = n, \ldots 2$, besides specifying that the basis vector ψ_λ belongs to the irrep (λ_f) of S_f, also gives the difference between the number of the symmetric bonds and the number of anti-symmetric bonds for the first f particles in the basis function $\psi_\lambda = \psi_m^{[\nu]}$. This can be shown as follows. In evaluating the expectation value of the transposition $(ij), \psi_m^{[\nu]}$ can be expressed in the following way

$$\psi_m^{[\nu]} = S_{ij}\psi_{ij}^{(s)} + A_{ij}\psi_{ij}^{(a)} ,$$

where $\psi_{ij}^{(s)}(\psi_{ij}^{(a)})$ stands for the wave function which is symmetric (anti-symmetric) in the indices i and j. Thus

$$\lambda_n^{(\nu)} = \sum_{i>j=1}^{n} (|S_{ij}|^2 - |A_{ij}|^2) = n_s - n_a . \tag{4-22}$$

For the totally symmetric (anti-symmetric) irrep, λ_n reaches the maximum (minimum) $(\lambda_n)_{\max} = \binom{n}{2}[(\lambda_n)_{\min} = -\binom{n}{2}]$.

Now let us find the relation between the eigenvalue $\lambda_n^{[\nu]}$ and the partition $[\nu]$. Let $Y_1^{[\nu]}$ be the Yamanouchi basis vector having the maximum Yamanouchi numbers. We split the 2-cycle class operator $C(n)$ into three parts

$$C(n) = \sum_{j\geq i=1}^{n} (ij) = T_r + T_c + T_m , \tag{4-23a}$$

where $T_r(T_c)$ is the sum of the transpositions i and j which are in the same rows (columns) of $Y_1^{[\nu]}$ and T_m is the remaining part of $C(n)$. Let A be the product of the anti-symmetrizers for the columns of $Y_1^{[\nu]}$. For instance, if

$$Y_1^{[\nu]} = \begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline 4 & 5 \\ \cline{1-2} 6 \\ \cline{1-1} \end{array}$$

then

$$A = \mathcal{A}(146)\mathcal{A}(25) ,$$

where $\mathcal{A}$ are anti-symmetrizers [see Eq. (4-68b)],

$$\mathcal{A}(i_1 i_2 \ldots i_n) = \frac{1}{n!}\sum_p \delta_p p , \quad p \in S_n(i_1 \ldots i_n) .$$

From

$$[C(n), A] = 0, \quad [T_c, A] = 0 , \tag{4-23b,c}$$

we have

$$[T_r + T_m,\ A] = 0 . \tag{4-23d}$$

Using Eq. (4-23d) we get

$$\begin{aligned} C(n)A|Y_1^{[\nu]}\rangle &= AT_r|Y_1^{[\nu]}\rangle + T_cA|Y_1^{[\nu]}\rangle + AT_m|Y_1^{[\nu]}\rangle \\ &= \left[\tfrac{1}{2}\sum_i \nu_i(\nu_i - 1) - \tfrac{1}{2}\sum_i \mu_i(\mu_i - 1)\right]A|Y_1^{[\nu]}\rangle + AT_m|Y_1^{[\nu]}\rangle , \end{aligned} \tag{4-24a}$$

where $[\mu_1\mu_2\ldots] = [\tilde{\nu}]$ is the partition conjugate to $[\nu]$. We are going to show next that $AT_m|Y_1^{[\nu]}\rangle$ is identically zero.

Suppose that i and j are two numbers in the same row of $Y_1^{[\nu]}$, and i and k are two numbers in the same column of $Y_1^{[\nu]}$. According to

$$\begin{array}{ccccccc} i\ldots j & & j\ldots i & & k\ldots i & & i\ldots k \\ \vdots & \xrightarrow{(ij)} & \vdots & \xrightarrow{(jk)} & \vdots & \xrightarrow{(ik)} & \vdots \\ k & & k & & j & & j \end{array}$$

we know that

$$(jk) = (ik)(jk)(ij) \ ,$$

where (ij) belongs to T_r, and (ik) belongs to T_c. Consequently, we have

$$A(jk)|Y_1^{[\nu]}\rangle = A(ik)(jk)(ij)|Y_1^{[\nu]}\rangle = A(ik)(jk)|Y_1^{[\nu]}\rangle = -A(jk)|Y_1^{[\nu]}\rangle \ ,$$

where the property $A(ik) = -A$ has been used. Thus we have shown that

$$A(jk)|Y_1^{[\nu]}\rangle = 0 \ ,$$

which implies that

$$AT_m|Y_1^{[\nu]}\rangle = 0 \ . \tag{4-24b}$$

From (4-24a) and (4-24b) and since $A|Y_1^{[\nu]}\rangle$ still belongs to the irrep $[\nu]$ (but is not a Yamanouchi basis vector) and since the eigenvalue $\lambda_n^{[\nu]}$ only depends on the irrep $[\nu]$, we get

$$\lambda_n^{[\nu]} = \frac{1}{2}\sum_i \nu_i(\nu_i - 1) - \frac{1}{2}\sum_i \mu_i(\mu_i - 1) \ . \tag{4-24c}$$

Comparing Eq. (4-22) with (4-24c) we infer that

$$n_s = \frac{1}{2}\sum_i \nu_i(\nu_i - 1) \ , \tag{4-24d}$$

$$n_a = \frac{1}{2}\sum_i \mu_i(\mu_i - 1) \ . \tag{4-24e}$$

We can rewrite n_a as

$$n_a = \frac{1}{2}\sum_{l=1}^{n}(\nu_l - \nu_{l+1})l(l-1). \tag{4-24f}$$

Substituting this into (4-24c) finally gives

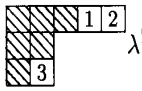
$$\lambda_n^{[\nu]} = \frac{1}{2}\sum_i \nu_l(\nu_l - 2l + 1) \ . \tag{4-25}$$

Equation (4-25) provides us with a simple method for calculating the eigenvalue associated with the Young diagram $[\nu]$. All the boxes in the same row (column) are regarded as symmetric (anti-symmetric), while the boxes which are neither in the same row nor the same column are counted as half symmetric and half anti-symmetric and thus do not contribute to $\lambda_n^{[\nu]}$.

2. From (4-9a) we know that the conjugate Young diagrams have opposite eigenvalues. Consequently self-conjugate Young diagrams correspond to zero eigenvalue:

$$\lambda_n^{[\nu]} = 0, \quad \text{if} \quad [\nu] = [\tilde{\nu}] \ .$$

The counting of n_s and n_a in a Young diagram $[\nu]$ can be further simplified by recognizing that a self-conjugate diagram inside the Young diagram $[\nu]$ does not contribute to $\lambda_n^{[\nu]}$. For example



$$\lambda^{[522]} = 0 + 3 + 4 + 1 - 2 = 6 \ .$$

The hatched diagram contributes zero. Adding successively box 1 and box 2 give three and four symmetric bonds, while adding box 3 gives 1 symmetric and 2 antisymmetric bond(s). Therefore $\lambda^{[522]} = 8 - 2 = 6$.

3. From Eq. (4-25) we know that associated with each basis vector ψ_λ, there is a basis vector $\psi_{-\lambda}$ where $-\lambda \equiv (-\lambda_n, -\lambda_{n-1}, \ldots, -\lambda_2)$. Since $\pm\lambda_n$ correspond to conjugate representations, ψ_λ and $\psi_{-\lambda}$ must belong to conjugate Young tableaux, that is

$$(\nu m) = (\lambda_n \ldots \lambda_2) \ , \quad (\tilde{\nu}\tilde{m}) = (-\lambda_n \ldots -\lambda_2) \equiv (\tilde{\lambda}_n \ldots \tilde{\lambda}_2) \ . \tag{4-26a}$$

For example one has

$$\psi_{3,2,2,3,1} = \begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4&5&6\\\hline\end{array} \ , \qquad \psi_{-3,-2,-2,-3,-1} = \begin{array}{|c|c|}\hline 1&4\\\hline 2&5\\\hline 3&6\\\hline\end{array} \ . \tag{4-26b}$$

4. The ψ_ν are orthonormal:

$$\begin{aligned} &\langle\psi_\lambda|\psi_{\lambda'}\rangle = \delta_{\lambda\lambda'} \ , \\ &\delta_{\lambda\lambda'} = \delta_{\lambda_n\lambda'_n}\delta_{\lambda_{n-1}\lambda'_{n-1}} \ldots \delta_{\lambda_2\lambda'_2} \ . \end{aligned} \tag{4-26c}$$

5. The enumeration of the Yamanouchi basis vectors according to the Yamanouchi symbols in decreasing page order, is equivalent to enumerating them according to the eigenvalues $(\lambda_n, \lambda_{n-1}, \ldots, \lambda_2)$ in decreasing page order.

According to the branching diagrams, such as Fig. 4.5-3, by taking a suitable linear combination of the $(n-1)$ 2–cycle class operators one can easily construct a single operator

$$M = \sum_{f=2}^{n} k_f C(f) \ , \tag{4-27a}$$

such that M is a CSCO–II of S_n . To this end, we only need to choose the coefficients k_f properly so as to make the eigenvalues λ of the operator M all distinct for each Yamanouchi basis vector of S_n,

$$\lambda = \sum_{f=2}^{n} k_f \lambda_f \ . \tag{4-27b}$$

For instance

$$M = \sum_{f=2}^{n} (f+7) C(f) \ , \tag{4-27c}$$

is a CSCO–II of S_n for $n \leq 6$.

Ex. 4.3. Give the three labelling schemes for the Yamanouchi basis vectors of the irrep [311].

4.6. The EFM for the Yamanouchi Basis (I)

The Yamanouchi basis can be found by solving the following eigenequations

$$\begin{pmatrix} C(n) \\ C(s) \end{pmatrix} \psi_m^{(\nu)} = \begin{pmatrix} \nu \\ m \end{pmatrix} \psi_m^{(\nu)} \ , \quad C(s) = \big(C(n-1), \ldots C(2)\big) \ . \tag{4-28a}$$

This may also be written as

$$\begin{aligned} &C(f)\psi_m^{(\nu)} = \lambda_f \psi_m^{(\nu)}, \quad f = n, n-1, \ldots, 2 \ . \\ &C(f) = \sum_{i>j=1}^{f} (ij) \ , \\ &\psi_m^{(\nu)} = \psi_\lambda, \quad \lambda = (\nu, m) = (\lambda_n, \lambda_{n-1}, \ldots, \lambda_2) \ , \end{aligned} \tag{4-28b}$$

or more concisely as

$$M\psi_\lambda = \lambda\psi_\lambda, \quad M = \big(C(n), C(n-1), \ldots C(2)\big) \ . \tag{4-28c}$$

If we take the single operator M in (4-27a) as the CSCO-II of S_n, then the problem of finding the Yamanouchi basis is reduced to that of solving the eigenequation of a single operator M,

$$M\psi_\lambda = \lambda\psi_\lambda \ , \quad M = \sum_{f=2}^{n} k_f C(f) \ . \tag{4-29}$$

For calculation by computer (4-29) is much simpler than (4-28). Nevertheless, for hand calculations, (4-28) is preferable. From now on, the eigenequations $M\psi_\lambda = \lambda\psi_\lambda$ can be understood either as (4-28) or (4-29).

In practical calculations, we often solve first the eigenequation of $C(2)$, and then solve the eigenequations of $C(3), \ldots, C(n)$ in the two eigenspaces of $C(2)$ with the eigenvalues $\lambda_2 = \pm 1$. Likewise, $C(3), \ldots, C(n)$ can be combined linearly into a single operator

$$M' = \sum_{f=3}^{n} a_f C(f) \ , \tag{4-30a}$$

such that all the eigenvalues of M' are different,

$$\lambda = \sum_{f=3}^{n} a_f \lambda_f \ . \tag{4-30b}$$

Solving the eigenequation of M' in the eigenspaces of $C(2)$ gives the Yamanouchi basis. For example, for $n \leq 6$ we can choose

$$M' = \sum_{f=3}^{n} (2f-5) C(f) \ , \quad \lambda = \sum_{f=3}^{n} (2f-5)\lambda_f \ . \tag{4-31}$$

Table 4.4-1 gives the eigenvalues λ of the Yamanouchi basis vectors with $\lambda_2 = 1$.

Example 1. Find the Yamanouchi basis of S_4 in the configuration $\alpha^3\beta$. The reducible basis vectors are

$$\varphi_1 = |\alpha\alpha\alpha\beta\rangle \ , \quad \varphi_2 = |\alpha\alpha\beta\alpha\rangle \ , \quad \varphi_3 = |\alpha\beta\alpha\alpha\rangle \ , \quad \varphi_4 = |\beta\alpha\alpha\alpha\rangle \ . \tag{4-32}$$

$$C(4) = \begin{pmatrix} 3 & 1 & 1 & 1 \\ 1 & 3 & 1 & 1 \\ 1 & 1 & 3 & 1 \\ 1 & 1 & 1 & 3 \end{pmatrix} \ , \quad C(3) = \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix} \ , \quad C(2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \ . \tag{4-33}$$

Using the elimination method discussed before, a simultaneous diagonalization of the three matrices of (4-33) gives the Yamanouchi bases of S_4,

$$\begin{aligned}
\psi_{6,3,1} &= \left|\begin{array}{|c|c|c|c|}\hline 1&2&3&4\\\hline\end{array}\right\rangle = \frac{1}{2}(\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4) \ , \\
\psi_{2,3,1} &= \left|\begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4\\\cline{1-1}\end{array}\right\rangle = \frac{1}{\sqrt{12}}(3\varphi_1 - \varphi_2 - \varphi_3 - \varphi_4) \ , \\
\psi_{2,0,1} &= \left|\begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array}\right\rangle = \frac{1}{\sqrt{6}}(2\varphi_2 - \varphi_3 - \varphi_4) \ , \\
\psi_{2,0,-1} &= \left|\begin{array}{|c|c|c|}\hline 1&3&4\\\hline 2\\\cline{1-1}\end{array}\right\rangle = \frac{1}{\sqrt{2}}(\varphi_3 - \varphi_4) \ .
\end{aligned} \tag{4-34}$$

In Sec. 3.13, it was pointed out that once we know one component of an irreducible basis, we can use (3-253) to obtain the other components. From Eqs. (4-17) and (4-14) one has

$$|Y^{[\nu]}_{m'}\rangle = \Big[\big(T - D^{[\nu]}_{mm}(T)\big)/D^{[\nu]}_{m'm}(T)\Big]|Y^{[\nu]}_{m}\rangle,$$
$$Y^{[\nu]}_{m'} = TY^{[\nu]}_{m}, \quad T = (i-1,i), \quad i = 2,3,\ldots n\ , \tag{4-35}$$

where $D^{[\nu]}_{m'm}(T)$ is given by (4-14). Comparing (4-35) with (3-253), it is seen that

$$F^{(\nu)}_{m'm} = \big(T - D^{(\nu)}_{mm}(T)\big)/D^{(\nu)}_{m'm}(T)\ . \tag{4-36a}$$

From the eigenequation (4-29) (or (4-28)) we can find τ_ν eigenvectors $\psi^{(\nu)\tau}_m$ where $\tau = 1,\ldots,\tau_\nu$, for a particular (ν,m). Choosing the appropriate adjacent permutations T and using the Yamanouchi matrix elements (4-14) (or Table 4.4-1 for S_n with $n \leq 5$), we find, from

$$\psi^{(\nu)}_{m'} = F^{(\nu)}_{m'm}\psi^{(\nu)\tau}_m\ , \tag{4-36b}$$

all the other components successively. For the irrep [32] of S_5, from the component $\left|\begin{smallmatrix}123\\45\end{smallmatrix}\right\rangle$, we can obtain all the other components by applying adjacent permutations in the following way

$$\left|\begin{matrix}1\,2\,3\\4\,5\end{matrix}\right\rangle \overset{(34)}{\to} \left|\begin{matrix}1\,2\,4\\3\,5\end{matrix}\right\rangle \overset{(23)}{\to} \left|\begin{matrix}1\,3\,4\\2\,5\end{matrix}\right\rangle \overset{(45)}{\to} \left|\begin{matrix}1\,3\,5\\2\,4\end{matrix}\right\rangle$$
$$\downarrow (45)$$
$$\left|\begin{matrix}1\,2\,5\\3\,4\end{matrix}\right\rangle .$$

The EFM for finding the Yamanouchi basis can be summarized as follows:

1. For a given configuration $(\alpha)^{n_1}(\beta)^{n_2}(\gamma)^{n_3}\ldots$ of an n-particle system, write down all possible n-particle product states $\varphi_a, a = 1,2,\ldots,N$, where

$$N = \frac{n!}{n_1!n_2!n_3!\ldots}\ . \tag{4-37}$$

2. Let $\psi_\lambda = \sum_a u_{\lambda a}\varphi_a$ be the required Yamanouchi basis, where $u_{\lambda a}$ are solutions of the following eigenequations

$$\sum_b \big(\langle\varphi_a|C(f)|\varphi_b\rangle - \lambda_f\delta_{ab}\big)u_{\lambda b} = 0\ ,$$
$$a = 1,2,\ldots,N, \quad f = n, n-1,\ldots,2\ . \tag{4-38}$$

Let us define $p_{if} = (if)$. Using

$$C(f) = C(f-1) + \sum_{i=1}^{f-1} p_{if}\ , \tag{4-39}$$

we can simplify Eq. (4-38) to

$$\sum_b \Big[\sum_{i=1}^{f-1}\langle\varphi_a|p_{if}|\varphi_b\rangle - (\lambda_f - \lambda_{f-1})\delta_{ab}\Big]u_{\lambda b} = 0\ , \quad f = 2,3,\ldots,n\ . \tag{4-40}$$

with the convention that $\lambda_1 \equiv 0$.

3. Use the branching diagram to choose an appropriate set of eigenvalues $(\lambda_2, \lambda_3, \ldots)$. Substitute those into (4-40) and solve (4-40) in the sequence $f = 2, 3, \ldots$

4. If the eigenvalue $\lambda = (\nu, m)$ has no degeneracy, (4-40) gives a unique solution $\psi_m^{(\nu)}$. If $\lambda = (\nu, m)$ has τ–fold degeneracy, we can get τ orthornormal solutions $\psi_m^{(\nu)1}, \ldots, \psi_m^{(\nu)\tau}$ from (4-40).

5. Use (4-36) to find all the other components of the Yamanouchi basis.

Example 2: Finding the Yamanouchi basis of S_4 for the configuration $\alpha^2\beta\gamma$. In this configuration there are $N = 12$ product states listed in the first column of Table 4.6-1. The indices of these states are given in the second column. The result of applying $C(12) = (12)$ to these 12 states is shown in the third column.

Table 4.6-1. Permutations acting on the product states.†*

φ_a	b / (ij) / a	(12)	(13)	(23)	(14)	(24)	(34)
$\|\alpha\alpha\beta\gamma\rangle$	1	1	2	3			6
$\|\beta\alpha\alpha\gamma\rangle$	2	3	1	2	7	11	8
$\|\alpha\beta\alpha\gamma\rangle$	3	2		1			10
$\|\gamma\alpha\beta\alpha\rangle$	4	5	8	12	1	4	7
$\|\alpha\gamma\beta\alpha\rangle$	5	4		10			9
$\|\alpha\alpha\gamma\beta\rangle$	6	6	7	9			1
$\|\gamma\alpha\alpha\beta\rangle$	7	9	6	7	2	12	4
$\|\beta\alpha\gamma\alpha\rangle$	8	10		11			2
$\|\alpha\gamma\alpha\beta\rangle$	9	7		6			5
$\|\alpha\beta\gamma\alpha\rangle$	10	8	12	5	10	6	3
$\|\beta\gamma\alpha\alpha\rangle$	11	12	5	8			11
$\|\gamma\beta\alpha\alpha\rangle$	12	11		4			12

†$(ij)\varphi_a = \varphi_b$.

*The blanks indicate that these entries are irrelevant to us here.

We only need to find the solution of one component for each irrep. For almost any irrep of S_n the value of λ_2 can be chosen arbitrarily, say $\lambda_2 = -1$. The exception is the totally symmetric irrep. Setting $\lambda_2 = -1$ we obtain, from the second and third columns of Table 4.6-1,

$$\lambda_2 = -1: \; u_2 = -u_3\,, \;\; u_4 = -u_5\,, \;\; u_7 = -u_9\,, \;\; u_{10} = -u_8\,, \;\; u_{11} = -u_{12}\,. \tag{4-41}$$

So the number of independent variables is reduced from 12 to 7. Out of the 12 we can choose 7 as independent variables; for example we may choose $u_1, u_2, u_4, u_6, u_7, u_{10}$ and u_{11}. Next, we solve the eigenequation of $C(3)$. From (3-75b) it is seen that to obtain the matrix elements of $C(3)$, we only need to apply the permutations (13) and (23) to the states $\varphi_1, \varphi_2, \varphi_4, \varphi_6, \varphi_7, \varphi_{10}$ and φ_{11}. The result is given in Table 4.6-1. From (3-75b) and the rows 1, 2, 4, 6 in Table 4.6-1 we get

$$\begin{aligned} &u_1 + u_2 + u_3 = \lambda_3 u_1\,, \quad u_3 + u_1 + u_2 = \lambda_3 u_2\,, \\ &u_5 + u_8 + u_{12} = \lambda_3 u_4\,, \quad u_6 + u_7 + u_9 = \lambda_3 u_6\,. \end{aligned} \tag{4-42a}$$

According to Fig. 4.5-3, apart from the totally symmetric and anti–symmetric irreps, any irrep of S_n has components with $\lambda_3 = 0$. From Eq. (4-42a) with $\lambda_3 = 0$, we get the three independent equations

$$u_1 + u_2 + u_3 = 0, \quad u_5 + u_8 + u_{12} = 0\,, \quad u_6 + u_7 + u_9 = 0\,. \tag{4-42b}$$

It is easy to check that the remaining rows 7, 10, 11 in Table 4.6-1 do not yield new equations. Combining (4-42b) and (4-41), we have

$$u_1 = u_6 = 0, \quad u_{12} = u_4 + u_{10} \ . \tag{4-43}$$

Therefore the seven independent variables are reduced to four, which can be chosen to be u_2, u_4, u_7 and u_{10}.

Similarly applying the permutations (14), (24) and (34) to $\varphi_2, \varphi_4, \varphi_7$ and φ_{10}, we get the result listed in Table 4.6-1. From (4-40) and rows 2,4,7,10 of Table 4.6-1, we get the eigenequation of $C(4)$ (noting that $\lambda_3 = 0$),

$$\begin{aligned} u_7 + u_{11} + u_8 = -u_4 + u_7 - 2u_{10} &= \lambda_4 u_2 \ , \\ u_1 + u_4 + u_7 = u_4 + u_7 &= \lambda_4 u_4 \ , \\ u_2 + u_{12} + u_4 = u_2 + 2u_4 + u_{10} &= \lambda_4 u_7 \ , \\ u_{10} + u_6 + u_3 = -u_2 + u_{10} &= \lambda_4 u_{10} \ . \end{aligned} \tag{4-44}$$

$$\begin{vmatrix} -\lambda_4 & -1 & 1 & -2 \\ 0 & 1-\lambda_4 & 1 & 0 \\ 1 & 2 & -\lambda_4 & 1 \\ -1 & 0 & 0 & 1-\lambda_4 \end{vmatrix} = \lambda_4(\lambda_4 - 2)^2(\lambda_4 + 2) = 0 \ . \tag{4-45}$$

Equation (4-45) tells us that the irrep $\lambda_4 = 0$ (corresponding to [22] from Table 3.2-1) and $\lambda_4 = -2$([211]) each occurs once and $\lambda_4 = 2$ ([31]) occurs twice. In the following we will find the solutions for each of the eigenvalues λ_4.

(a) $\lambda_4 = 0$: Substituting $\lambda_4 = 0$ into (4-44), we obtain ratios between u_2, u_4, u_7 and u_{10}. Using (4-41) and (4-43), we have[1)]

$$\psi_{0,0,-1} = \left| \begin{array}{|c|c|}\hline 1&3\\\hline 2&4\\\hline\end{array} \ \begin{array}{|c|c|}\hline \alpha&\alpha\\\hline \beta&\gamma\\\hline\end{array} \right\rangle = \frac{1}{\sqrt{8}}[\varphi_3 + \varphi_4 + \varphi_8 + \varphi_9 - \varphi_2 - \varphi_5 - \varphi_7 - \varphi_{10}] \ . \tag{4-46a}$$

From (4-36) and the fifth column of Table 4.6-1, as well as the matrix elements of the irrep [22] in Table 4.4-2, we obtain another component of the irrep [22]

$$\begin{aligned} \psi_{0,0,1} &= \left| \begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\hline\end{array} \ \begin{array}{|c|c|}\hline \alpha&\alpha\\\hline \beta&\gamma\\\hline\end{array} \right\rangle = [(23) - D^{[22]}_{22}(23)]\psi^{(0)}_{0,-1} / D^{[22]}_{12}(23) = \left[(23) - \frac{1}{2}\right] \psi^{(0)}_{0,-1} \Big/ \frac{\sqrt{3}}{2} \\ &= \frac{1}{\sqrt{24}}[2(\varphi_1 + \varphi_6 + \varphi_{11} + \varphi_{12}) - (\varphi_2 + \varphi_3 + \varphi_4 + \varphi_5 + \varphi_7 + \varphi_8 + \varphi_9 + \varphi_{10})] \ . \end{aligned} \tag{4-46b}$$

(b) $\lambda_4 = -2$: Similarly we find

$$\begin{aligned} \psi_{-2,0,-1} = \left| \begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1} 4\\\cline{1-1}\end{array} \ \begin{array}{|c|c|}\hline \alpha&\alpha\\\hline \beta\\\cline{1-1} \gamma\\\cline{1-1}\end{array} \right\rangle &= \frac{1}{\sqrt{48}}[3(\varphi_3 - \varphi_2 + \varphi_7 - \varphi_9) \\ &\quad + 2(\varphi_{11} - \varphi_{12}) + (-\varphi_4 + \varphi_5 + \varphi_8 - \varphi_{10})] \ , \end{aligned}$$

[1)] The *Weyl tableaux*, like $\begin{array}{|c|c|}\hline \alpha&\alpha\\\hline \beta&\gamma\\\hline\end{array}$ will not be used until Sec. 4.8.

$$\psi_{-2,0,1} = \left| \begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1} 4\\\cline{1-1}\end{array} \quad \begin{array}{|c|c|}\hline \alpha&\alpha\\\hline \beta\\\cline{1-1} \gamma\\\cline{1-1}\end{array} \right\rangle = [(23) - D_{22}^{[211]}(23)]\psi_{0,-1}^{(-2)}/D_{12}^{[211]}(23)$$

$$= \frac{1}{\sqrt{16}}[2(\varphi_1 - \varphi_6) - (\varphi_2 + \varphi_3 + \varphi_4 + \varphi_5) + (\varphi_7 + \varphi_8 + \varphi_9 + \varphi_{10})] ,$$

$$\psi_{-2,-3,-1} = \left| \begin{array}{|c|c|}\hline 1&4\\\hline 2\\\cline{1-1} 3\\\cline{1-1}\end{array} \quad \begin{array}{|c|c|}\hline \alpha&\alpha\\\hline \beta\\\cline{1-1} \gamma\\\cline{1-1}\end{array} \right\rangle = [(34) - D_{22}^{[211]}(34)]\psi_{0,-1}^{(-2)}/D_{32}^{[211]}(34)$$

$$= \frac{1}{\sqrt{6}}(\varphi_4 + \varphi_{10} + \varphi_{11} - \varphi_5 - \varphi_8 - \varphi_{12}) . \tag{4-47}$$

(c) $\lambda_4 = 2$: This is a double root. From (4-44), we obtain only two independent equations

$$u_4 = u_7 , \quad u_2 = -u_{10} . \tag{4-48a, b}$$

The solutions of (4-48) are not unique. We may for example choose $(u_2, u_4) = (0,1)$ and $(1,0)$, and obtain the following two solutions

$$\psi_{2,0,-1}^{\tau} = \left| \begin{array}{|c|c|c|}\hline 1&3&4\\\hline 2\\\cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline \alpha&\alpha&\beta\\\hline \gamma\\\cline{1-1}\end{array} \right\rangle = \frac{1}{\sqrt{6}}(-\varphi_4 + \varphi_5 - \varphi_7 + \varphi_9 + \varphi_{11} - \varphi_{12}) , \tag{4-49a}$$

$$\psi'^{(2)\theta}_{0,-1} = \frac{1}{\sqrt{6}}(\varphi_2 - \varphi_3 + \varphi_8 - \varphi_{10} + \varphi_{11} - \varphi_{12}) . \tag{4-49b}$$

After orthogonalization, the second solution becomes

$$\psi_{2,0,-1}^{\theta} = \left| \begin{array}{|c|c|c|}\hline 1&3&4\\\hline 2\\\cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline \alpha&\alpha&\gamma\\\hline \beta\\\cline{1-1}\end{array} \right\rangle = N\left[\psi'^{\theta}_{2,0,-1} - \langle\psi^{\tau}_{2,0,-1}|\psi'^{\theta}_{2,0,-1}\rangle\psi^{\tau}_{2,0,-1}\right]$$

$$= \frac{1}{\sqrt{48}}[3(-\varphi_2 + \varphi_3 - \varphi_8 + \varphi_{10}) - 2(\varphi_{11} - \varphi_{12}) + (-\varphi_4 + \varphi_5 - \varphi_7 + \varphi_9)] . \tag{4-49c}$$

From (4-36) and the Yamanouchi matrix elements of [31] in Table 4.4-2, we obtain the remaining components

$$\psi_{2,3,1}^{\tau} = \left| \begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4\\\cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline \alpha&\alpha&\beta\\\hline \gamma\\\cline{1-1}\end{array} \right\rangle = \frac{1}{6}\left[3(\varphi_1 + \varphi_2 + \varphi_3) - \sum_{a=4}^{12}\varphi_a\right] ,$$

$$\psi_{2,3,1}^{\theta} = \left| \begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4\\\cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline \alpha&\alpha&\gamma\\\hline \beta\\\cline{1-1}\end{array} \right\rangle = \frac{1}{\sqrt{18}}[2(\varphi_6 + \varphi_7 + \varphi_9) - (\varphi_4 + \varphi_5 + \varphi_8 + \varphi_{10} + \varphi_{11} + \varphi_{12})] ,$$

$$\psi_{2,0,1}^{\tau} = \left| \begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline \alpha&\alpha&\beta\\\hline \gamma\\\cline{1-1}\end{array} \right\rangle = \frac{1}{\sqrt{18}}[2(\varphi_6 + \varphi_8 + \varphi_{10}) - (\varphi_4 + \varphi_5 + \varphi_7 + \varphi_9 + \varphi_{11} + \varphi_{12}] ,$$

$$\psi_{2,0,1}^{\theta} = \left| \begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline \alpha&\alpha&\gamma\\\hline \beta\\\cline{1-1}\end{array} \right\rangle = \frac{1}{12}[3(2\varphi_1 - \varphi_2 - \varphi_3) - 4(\varphi_{11} + \varphi_{12})$$

$$+ 5(\varphi_4 + \varphi_5) + 2\varphi_6 - (v p_7 + \varphi_8 + \varphi_9 + \varphi_{10})] . \tag{4-49d}$$

We started with 12 reducible basis vectors, and have already found 11 irreducible basis vectors. The one left over must belong to either the totally symmetric or anti-symmetric irrep. Starting from (4-41), we found all solutions corresponding to $\lambda_2 = -1$. Consequently, the one which is left over must belong to $\lambda_2 = 1$, that is to the totally symmetric irrep. We can write this irreducible basis down immediately as

$$\psi_{6,3,1} = \left| \boxed{1}\boxed{2}\boxed{3}\boxed{4} \quad \boxed{\alpha}\boxed{\alpha}\boxed{\beta}\boxed{\gamma} \right\rangle = \frac{1}{\sqrt{12}} \sum_{a=1}^{12} \varphi_a \ . \tag{4-50}$$

Supposing that the wave functions of the single particle states α, β and γ are proportional to 1, x and y respectively, from (4-46) and (4-47) we have

$$\begin{aligned}
\psi_{0,0,1} &= \left| \begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\hline\end{array} \right\rangle = [2x_1y_2 + 2x_3y_4 - (x_1+x_2)(y_3+y_4)] + [x \leftrightarrow y] \ , \\
\psi_{0,0,-1} &= \left| \begin{array}{|c|c|}\hline 1&3\\\hline 2&4\\\hline\end{array} \right\rangle = [(x_1-x_2)(y_3-y_4)] + [x \leftrightarrow y] \ , \\
\psi_{-2,0,1} &= \left| \begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1} 4\\\cline{1-1}\end{array} \right\rangle = [(x_1+x_2)y_3 - (x_1+x_2-2x_3)y_4] - [x \leftrightarrow y] \ , \\
\psi_{-2,0,-1} &= \left| \begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1} 4\\\cline{1-1}\end{array} \right\rangle = [(x_1-x_2)(y_3-3y_4) + 2x_1y_2] - [x \leftrightarrow y] \ , \\
\psi_{-2,-3,-1} &= \left| \begin{array}{|c|c|}\hline 1&4\\\hline 2\\\cline{1-1} 3\\\cline{1-1}\end{array} \right\rangle = \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix} \ .
\end{aligned} \tag{4-51}$$

Here $[x \leftrightarrow y]$ denotes an interchange of x and y in the previous term.[2)]

4.7. The CSCO-III of the Permutation Group

4.7.1. CSCO-III

According to Secs. 3.8 and 4.5, we know that the CSCO-III of S_n consists of $(2n-3)$ 2-cycle class operators

$$K = (C(n), C(n-1), C(n-2), \ldots C(2), \overline{C}(n-1),\ \overline{C}(n-2)\ , \ldots \overline{C}(2)) \ , \tag{4-52a}$$

where $\overline{C}(f)$ is the 2-cycle class operator of the intrinsic permutation group $\overline{S}_f$.

In the space spanned by n-particle product states, it is more convenient to use the following operator as the CSCO-III,

$$K = (C(n), C(n-1), \ldots, C(2), \mathcal{C}(n-1), \ldots, \mathcal{C}(2)) \ , \tag{4-52b}$$

where $\mathcal{C}(f)$ is the 2-cycle class operator of the state permutation group $\mathcal{S}_f$.

The problem of decomposing the regular representation of S_n is converted into that of solving the eigenequation of the operator K. To see this, let $\psi_m^{(\nu)k}$ be the irreducible basis

$$\psi_m^{(\nu)k} = \sum_{a=1}^{n!} u_{\nu mk,a} \varphi_a \ , \tag{4-53a}$$

which satisfy the eigenequations

$$\begin{pmatrix} C(n) \\ C(s) \\ \overline{C}(s) \end{pmatrix} \psi_m^{(\nu)k} = \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} \psi_m^{(\nu)k} \ . \tag{4-53b}$$

[2)] The result for the first two basis vectors of the irrep [211] given in Bohr (1969) Section IC is incorrect.

$$C(s) = \big(C(n-1),\ldots,C(2)\big), \quad \overline{C}(s) = \big(\overline{C}(n-1),\ldots,\overline{C}(2)\big) ,$$
$$\nu = \lambda_n , \quad m = (\lambda_{n-1},\ldots,\lambda_2) , \quad k = (\overline{\lambda}_{n-1},\ldots,\overline{\lambda}_2) .$$

From Eqs. (4-53a) and (4-53b), we obtain the eigenequations satisfied by $u_{\nu mk,a}$,

$$\begin{aligned} &\sum_b K_{ab} u_{\lambda b} = \lambda u_{\lambda a} \\ &K_{ab} = \langle \varphi_a | K | \varphi_b \rangle, \quad \lambda = (\nu, m, k) . \end{aligned} \tag{4-53c}$$

In analogy with (4-29), the $(2n-3)$ 2–cycle class operators in (4-52a) can be combined into a single operator K such that it is a CSCO–III of S_n,

$$K = \sum_{f=2}^{n} a_f C(f) + \sum_{f=2}^{n-1} \overline{a}_f \overline{C}(f) . \tag{4-54}$$

This reduces the problem of simultaneously diagonalizing the $(2n-3)$ operators to that of diagonalizing a single operator. The operator K in (4-53c) can now be understood either as a set of $2n-3$ operators or as just a single operator (4-54).

For example, the CSCO-III of S_3 can be chosen as

$$K = 3C(3) + 2C(2) + \overline{C}(2) . \tag{4-55}$$

The operator K has six distinct eigenvalues 12, -12, 3, 1, -1, -3, corresponding to (ν, m, k) = (3, 1, 1), (-3, -1, -1), (0, 1, 1), (0, 1, -1), (0, -1, 1), (0, -1, -1) respectively. From Eqs. (4-55), (3-96) and (3-136), we obtain the representative of the operator K in the regular representation,

$$K = \begin{pmatrix} 0 & 6 & 3 & 3 & 0 & 0 \\ 6 & 0 & 0 & 0 & 3 & 3 \\ 3 & 0 & 0 & 0 & 4 & 5 \\ 3 & 0 & 0 & 0 & 5 & 4 \\ 0 & 3 & 4 & 5 & 0 & 0 \\ 0 & 3 & 5 & 4 & 0 & 0 \end{pmatrix} . \tag{4-56}$$

A diagonalization of K leads to (3-119).

4.7.2. The labelling for the Yamanouchi basis of S_n and $\mathcal{S}_n$

The *Yamanouchi basis* $\psi_m^{(\nu)k}$ of S_n and $\mathcal{S}_n$ (or $\overline{S}_n$) can be labelled by the $2n-3$ quantum numbers, among which the $(\nu, m) = (\lambda_n, \lambda_{n-1}, \ldots, \lambda_2)$ characterize the transformation property of the basis under S_n and the $(\nu, k) = (\lambda_n, \overline{\lambda}_{n-1}, \ldots, \overline{\lambda}_2)$ characterize the transformation property of the basis under $\mathcal{S}_n$ (or $\overline{S}_n$). As we mentioned in Sec. 4.5, the quantum numbers (ν, m), the Yamanouchi symbol $(r_n r_{n-1} \ldots r_2)$, and the Young tableau $Y_m^{[\nu]}$ are all equivalent to one another. Obviously, we can let the quantum number (ν, k) correspond to another Yamanouchi symbol $(\overline{r}_n \overline{r}_{n-1} \ldots \overline{r}_2)$, or another Young tableau $Y_k^{[\nu]}$. It follows that we have three equivalent ways for labelling the irreducible basis of S_n and $\overline{S}_n$:

1. Two sets of quantum numbers, (ν, m) and (ν, k),
2. Two sets of Yamanouchi symbols $(r_n \ldots r_2)$ and $(\overline{r}_n \ldots \overline{r}_2)$,
3. Two Young tableaux $Y_m^{[\nu]}$ and $Y_k^{[\nu]}$.

Since the Yamanouchi basis of the intrinsic group $\overline{S}_n$ is the Yamanouchi basis of the state permutation group $\mathcal{S}_n$, which can be labelled by the *Weyl tableau* $W_k^{(\nu)}$. One obtains $W_k^{(\nu)}$ by replacing the letter a in the Young tableau $Y_k^{(\nu)}$ by the state index $i_a, a = 1, 2, \ldots, n$. Clearly the Yamanouchi basis $|W_k^{(\nu)}\rangle$ of $\mathcal{S}_n$ and the Yamanouchi basis $|Y_k^{(\nu)}\rangle$ of $\overline{S}_n$ have the same properties, namely, $|W_k^{(\nu)}\rangle$ is symmetric (antisymmetric) with respect to two adjacent state indices which

are in the same row (column) and is neither symmetric nor anti-symmetric in all other cases. Thus, if $i_1 = \alpha, i_2 = \beta, i_3 = \gamma$ and $i_4 = \delta$, then $|^{\alpha\beta\gamma}_{\delta}\rangle$ is symmetric in the indices α, β, γ but has no symmetry with respect to the indices γ and δ. Therefore we have the fourth labelling scheme.

4. A Young tableau $Y_m^{(\nu)}$ and a Weyl tableau $W_k^{(\nu)}$.

4.7.3. The phase convention and the principal term

In order that the eigenvectors $\psi_m^{(\nu)k}$ of (4-53) satisfy the Yamanouchi phase convention, we must give a rule for choosing the phase of $\psi_m^{(\nu)k}$.

Let R_{mk} be a permutation operator which transfers the Young tableau $Y_k^{(\nu)}$ to the Young tableau $Y_m^{(\nu)}$,

$$Y_m^{(\nu)} = R_{mk} Y_k^{(\nu)} . \tag{4-57}$$

R_{mk} must be expressible in terms of the adjacent permutations

$$R_{mk} = T_\alpha T_\beta \dots T_\delta . \tag{4-58}$$

From (4-17) and (4-58) we have

$$\begin{aligned} D^{(\nu)}_{mk}(R_{mk}) &= \sum_{st\dots u} D^{(\nu)}_{ms}(T_\alpha) D^{(\nu)}_{st}(T_\beta) \dots D^{(\nu)}_{uk}(T_\delta) \\ &= D^{(\nu)}_{mi}(T_\alpha) D^{(\nu)}_{ij}(T_\beta) \dots D^{(\nu)}_{lk}(T_\delta) > 0 , \end{aligned} \tag{4-59a}$$

where[3)]

$$Y_l = T_\delta Y_k, \dots , \quad Y_i = T_\beta Y_j , \quad Y_m = T_\alpha Y_i .$$

According to the Yamanouchi phase convention (4-14b), the non-diagonal matrix elements of adjacent permutations in (4-59a) are all positive; therefore

$$D^{(\nu)}_{mk}(R_{mk}) > 0 . \tag{4-59b}$$

Equation (4-59b) gives the rule for determining the phase of the eigenvector

$$\mathbf{u}_{\nu mk} = (u_{\nu mk,1}, u_{\nu mk,2}, \dots, u_{\nu mk,g}) .$$

According to the quantum numbers (νm) and (νk), we determine the Young tableaux $Y_m^{(\nu)}$ and $Y_k^{(\nu)}$. Clearly there is one and only one operator $R_{a_0} = R_{mk}$ satisfying (4-57). Adjust the overall phase of the vector $\mathbf{u}_{\nu mk}$ so that the term $u_{\nu mk,a_0} > 0$. Such a term will be called the *principal term.* In Table 4.9, the framed terms are the principal terms. With n-particle product states as the reducible basis, it is easy to know which term is the principal term a_0 in $\psi_m^{(\nu)k} = |Y_m^{(\nu)}, W_k^{(\nu)}\rangle = \sum_a u_{\nu mk,a}\varphi_a$. For example, for the irreducible basis vector

$$\left| \begin{array}{|c|c|c|} \hline 1 & 2 & 4 \\ \hline 3 & 5 \\ \cline{1-2} 6 \\ \cline{1-1} \end{array} \quad \begin{array}{|c|c|c|} \hline \alpha & \gamma & \phi \\ \hline \beta & \delta \\ \cline{1-2} \epsilon \\ \cline{1-1} \end{array} \right\rangle , \quad \text{the principal term is } \varphi_{a_0} = |\alpha\gamma\beta\phi\delta\varepsilon\rangle . \tag{4-60}$$

It can be shown that the rule (4-60) for determining the principal term applies also to the case where there are identical single particle states in the Weyl tableau; see Table 4.9. It is easy to check that all the irreducible bases of S_3 and S_4 obtained in the previous sections fulfill this simple phase rule.

[3)] Notice that there is no summation index any more. From (4-14b) we have that $D^{(\nu)}_{mj}(T_\beta)=0$ for $Y_m^{(\nu)} \neq T_\beta Y_j^{(\nu)}$.

4.7.4. The matrix elements of conjugated irreps

Since the CSCO–III consists of 2-cycle class operators, the permutation parity of K is negative. Therefore

$$K_{ab} = 0, \quad \text{when} \quad \delta_a \delta_b \neq -1 \,, \tag{4-61}$$

where δ_a is the parity of the permutation p_a, as defined in (1-11). From (4-53c) and (4-61) one has

$$\sum_{b=1}^{g} K_{ab}(\delta_b u_{\lambda b}) = (-\lambda)(\delta_a u_{\lambda a}) \,. \tag{4-62}$$

This means that if $\{u_{\lambda a}\}$ is a solution corresponding to the eigenvalue λ, then there must exist a solution

$$u_{-\lambda a} = \pm \delta_a u_{\lambda a} \,, \tag{4-63}$$

corresponding to the eigenvalue $-\lambda$. From Sec. 4.5 we know that ψ_λ and $\psi_{-\lambda}$ are conjugate bases, that is if

$$\psi_\lambda = \psi_m^{(\nu)k} = |Y_m^\nu, Y_k^\nu\rangle = \sum_a u_{\lambda a}\varphi_a \,, \tag{4-64a}$$

then

$$\psi_{-\lambda} \equiv \psi_{\tilde{m}}^{(\tilde{\nu})\tilde{k}} = |\tilde{Y}_m^\nu, \tilde{Y}_k^\nu\rangle = \sum_a u_{-\lambda a}\varphi_a \,, \tag{4-64b}$$

where $-\lambda = (-\nu, -m, -k) = (\tilde{\nu}, \tilde{m}, \tilde{k})$. The Young tableaux $\tilde{Y}_m^{(\nu)} \equiv Y_{\tilde{m}}^{(\tilde{\nu})}$ and $\tilde{Y}_k^{(\nu)} \equiv Y_{\tilde{k}}^{(\tilde{\nu})}$ are the conjugate Young tableaux of $Y_m^{(\nu)}$ and $Y_k^{(\nu)}$, respectively.

The choice of the sign in (4-63) is determined by the phase convention. We use the Young–Yamanouchi phase convention which requires that the principal term $u_{\lambda a_0}$ be positive. If $Y_m = R_{mk}Y_k$, then $\tilde{Y}_m = R_{mk}\tilde{Y}_k$. This means that if $u_{\lambda a_0}$ is the principal term in ψ_λ, then $u_{-\lambda a_0}$ is the principal term in $\psi_{-\lambda}$. In order that $u_{-\lambda a_0} > 0$, (4-63) must take the following form

$$u_{-\lambda a} = \delta_{a_0}\delta_a u_{\lambda a} \,. \tag{4-65}$$

Since $D_{mk}^{(\nu)}(R_a) = \sqrt{g/h_\nu}u_{\nu mk,a}^*$, (4-65) can be rewritten as

$$D_{-m-k}^{(-\nu)}(R_a) = \delta_{a_0}\delta_a D_{mk}^{(\nu)}(R_a), \quad R_{a_0} = R_{mk} \,. \tag{4-66a}$$

A Young tableau $Y_m^{(\nu)}$ can be obtained from the Young tableau $Y_1^{(\nu)}$ (with the maximum Yamanouchi symbol) through a unique permutation $p, Y_m^{(\nu)} = pY_1^{(\nu)}$. To each Young tableau $Y_m^{(\nu)}$, we associate a phase factor $\Lambda_m^\nu = \delta_p$.

Equation (4-57) now requires that

$$\delta_{a_0} = \Lambda_m^\nu \Lambda_k^\nu \,. \tag{4-66b}$$

Inserting this into (4-66a) we obtain the relationship between the matrix elements of the irrep (ν) and its conjugate $(\tilde{\nu})$,[4)]

$$D_{\tilde{m}\tilde{k}}^{(\tilde{\nu})}(R_a) = \delta_a \Lambda_m^\nu \Lambda_k^\nu D_{mk}^{(\nu)}(R_a) \,. \tag{4-67}$$

4.7.5. The symmetrizer and anti-symmetrizer

The eigenvectors $P_{mk}^{[\nu]}$ in the group space of the CSCO–III of S_n are called the *orthogonal unit* $O_{mk}^{[\nu]}$ (Rutherford 1948),

$$P_{mk}^{[\nu]} = O_{mk}^{[\nu]} = \frac{h_\nu}{n!}\sum_a D_{mk}^{[\nu]}(p_a)p_a \,. \tag{4-68a}$$

[4)] Under Jahn's (1950) phase convention, $D_{\tilde{m}\tilde{k}}^{(\tilde{\nu})}(R_a) = \delta_a D_{mk}^{(\nu)}(R_a)$.

$P^{[n]}$ and $P^{[1^n]}$ are called the symmetrizer and anti-symmetrizer respectively. They are denoted by

$$\mathcal{S} = \frac{1}{n!}\sum_{a=1}^{n!} p_a, \quad \mathcal{A} = \frac{1}{n!}\sum_{a=1}^{n!} \delta_a p_a \ . \tag{4-68b}$$

4.8. The Quasi-Standard Basis of the Permutation Group

4.8.1 State permutation group (for the case with repeated state labels)

In Secs. 3.5 and 4.7 we discussed the state permutation group $\mathcal{S}_n$ for the case when there were n particles occupying n distinct single particle states. However, in physical applications, we deal more often with cases corresponding to n particles occupying $l < n$ single particle states. For example, consider an n-particle system in the configuration $(m_1)^{n_1}(m_2)^{n_2}\ldots(m_l)^{n_l}$ where $\sum_i n_i = n$. To define a state permutation for the cases with repeated state labels, we assign the l state labels $m_1, m_2, \ldots, m_l$ to the n state indices in the following way:

$$i_1 = \ldots = i_{n_1} = m_1, \quad i_{n_1+1} = \ldots = i_{n_1+n_2} = m_2, \ldots, \quad i_{n-n_l+1} = \ldots = i_n = m_l \ , \tag{4-69a}$$

That is the indices $1\ldots, n_1$ correspond to $m_1; n_1+1, \ldots, n_1+n_2$ correspond to $m_2, \ldots$, and $n-n_l+1, \ldots, n$ correspond to m_l.

As in the case without repeated state labels, the permutation operator $\wp$ of the state permutation group $\mathcal{S}_n$ is defined by

$$\wp_{ab}|\ldots i_a \ldots i_b \ldots\rangle = |\ldots i_b \ldots i_a \ldots\rangle \ . \tag{4-69b}$$

When there are no repeated state labels, that is for the configuration $(m_1)^1(m_2)^1\ldots(m_n)^1$, each single particle state m_a corresponds to a unique state index i_a. Therefore the meaning of state permutations is unambiguous. For the case with repeated state labels, for example, in the configuration $(m_1)^{n_1}(m_2)^{n_2}\ldots(m_l)^{n_l}$, a single particle state may correspond to several state indices. At the beginning we can specify the state indices in a *normal order state* $|\omega\rangle$ in the following way

$$\begin{aligned} &|m_1 \ldots m_1,\ m_2 \ldots m_2,\ \ldots,\ m_l \ldots m_l\rangle \\ \equiv |\omega\rangle &= |i_1 \ldots i_{n_1}, i_{n_1+1} \ldots\ i_{n_1+n_2},\ \ldots i_{n-n_l+1}, \ldots i_n\rangle \ . \end{aligned} \tag{4-70a}$$

Applying the $n!$ state permutations to $|\omega\rangle$, we can get N linearly independent states with

$$N = n!/(n_1!n_2!\ldots n_l!) \ . \tag{4-70b}$$

Among them, one is the normal order state, while the remaining $N-1$ are non-normal order states. For these non-normal order states, we are no longer able to distinguish which m_1 corresponds to i_1, which m_1 corresponds to $i_2, \ldots$, which m_2 corresponds to $i_{n_1+1}, \ldots$, and so on. So the meaning of state permutation is ambiguous.

This is not surprising if we remember that the state permutation group is a realization of the intrinsic permutation group $\overline{S}_n$ and that with the normal order state (4-70a) as the intrinsic state, single intrinsic group elements lose meaning. Only the CSCO of the group $\overline{S}_n$ and the CSCO of some subgroups of $\overline{S}_n$ still retain a definite meaning. In Sec. 3.13 we described a method for finding these meaningful operators.

The symmetry group of the intrinsic state $|\omega\rangle$ of (4-70a) is

$$G_{in} = S_{n_1}(1, \ldots, n_1) \times S_{n_2}(n_1+1, \ldots, n_1+n_2) \times \ldots \times S_{n_l}(n-n_l+1, \ldots n) \ .$$

The operators which commute with one another and with G_{in} are[5)]

[5)] In this section $C(i)$ stands for the CSCO of S_i rather than for the 2-cycle class operator of S_i.

$$(C, C(s')) = (C(n), C(n-n_l), \ldots, C(n_1+n_2), C(n_1)) \ . \tag{4-71a}$$

Therefore the CSCO, $(\overline{C}, \overline{C}(s'))$, and in turn the CSCO

$$(\mathcal{C}, \mathcal{C}(s')) = (\mathcal{C}(n), \mathcal{C}(n-n_l), \ldots, \mathcal{C}(n_1+n_2), \mathcal{C}(n_1)) \tag{4-71b}$$

of the group chain $\mathcal{S}_n \supset \mathcal{S}_{n-n_l} \supset \ldots \supset \mathcal{S}_{n_1+n_2} \supset \mathcal{S}_{n_1}$ have a definite meaning. In other words, the result of the action of any operator in (4-71b) is independent of which m_1 is regarded as i_1 which m_1 is regarded as $i_2, \ldots$, and which m_2 is regarded as i_{n_1+1}, and so on. For example, for the configuration $(\alpha)(\beta)^2(\gamma)$ $(i_1 = \alpha, i_2 = i_3 = \beta, i_4 = \gamma)$,

$$\mathcal{C}(3)|\beta\alpha\beta\gamma\rangle = \mathcal{C}(3)|i_2 i_1 i_3 i_4\rangle = \mathcal{C}(3)|i_3 i_1 i_2 i_4\rangle = |\beta\beta\alpha\gamma\rangle + |\beta\alpha\beta\gamma\rangle + |\alpha\beta\beta\gamma\rangle \ . \tag{4-72}$$

Equation (4-72) shows that the action of $\mathcal{C}(3)$ is independent of which β is assigned as i_2 or i_3.

4.8.2. The quasi-standard basis of the permutation group

The group chain $\mathcal{S}_n \supset \mathcal{S}_{n-n_l} \supset \ldots \supset \mathcal{S}_{n_1+n_2} \supset \mathcal{S}_{n_1}$ will be called a *broken chain* , in contrast to the "perfect chain" $\mathcal{S}_n \supset \mathcal{S}_{n-1} \supset \ldots \supset \mathcal{S}_2$. The broken chain is not canonical, since in the irreducible space (ν) with dimension h_ν, the CSCO of the broken chain, $(\mathcal{C}, \mathcal{C}(s'))$, only has $\tau_\nu < h_\nu$ sets of eigenvalues. Following Sec. 3.13.2, we call the simultaneous eigenfunctions $\psi^{(\nu)\kappa}$ of $(\mathcal{C}, \mathcal{C}(s'))$ the quasi-irreducible basis in the $G \supset G(s')$ classification. The eigenfunctions $\psi^{(\nu)\kappa}$ satisfy the following eigenequations

$$\begin{pmatrix} \mathcal{C} \\ \mathcal{C}(s') \end{pmatrix} \psi^{(\nu)\kappa} = \begin{pmatrix} \nu \\ \kappa \end{pmatrix} \psi^{(\nu)\kappa}, \quad \kappa = \kappa_1, \ldots, \kappa_{\tau_\nu} \ , \tag{4-73a}$$

$$\mathcal{C}(s') = (\mathcal{C}(n-n_l), \ldots, \mathcal{C}(n_1+n_2), \mathcal{C}(n_1)) \ , \tag{4-73b}$$

$$\kappa = (\overline{\lambda}(n-n_l), \ldots, \overline{\lambda}(n_1+n_2), \overline{\lambda}(n_1)) \ . \tag{4-73c}$$

The $\psi^{(\nu)\kappa}$ are referred to as the *quasi-standard basis* of the state permutation group $\mathcal{S}_n$. The quasi-standard basis $\psi^{(\nu)\kappa}$ is orthogonal in the quantum numbers ν and κ; however

$$\wp\psi^{(\nu)\kappa} \neq \sum_{\kappa'} D^{(\nu)}_{\kappa'\kappa}(p)\psi^{(\nu)\kappa'} \ , \tag{4-74}$$

since a single group element $\wp$ of $\mathcal{S}_n$ does not have a definite action on $\psi^{(\nu)\kappa}$.

Because the n_1–single particle state $|m_1 \ldots m_1\rangle$ must belong to the totally symmetric rep of the state permutation group $\mathcal{S}_{n_1}$, $\mathcal{C}(n_1)$ can be taken as the 2–cycle class operator $\mathcal{C}_{(2)}(n_1)$. Thus the eigenvalue of $\mathcal{C}_{(2)}(n_1)$ is simply

$$\overline{\lambda}(n_1) = \tfrac{1}{2} n_1(n_1 - 1) \ .$$

The method for decomposing a non–regular rep of S_n can be summarized as follows:

The eigenfunctions of the standard basis (ν, m) of S_n and of the quasi–standard basis (ν, κ) of $\mathcal{S}_n$ are expanded in terms of the N linearly independent basis vectors φ_a generated from $|\omega\rangle$,

$$\psi^{(\nu)\kappa}_m = \sum_{a=1}^{N} u_{\nu m \kappa, a}\varphi_a \ , \tag{4-75a}$$

$$\varphi_a = p_a|\underbrace{m_1 \ldots m_1}_{n_1}, \ldots, \underbrace{m_l \ldots m_l}_{n_l}\rangle = p_a|\omega\rangle \ . \tag{4-75b}$$

The $\psi_m^{(\nu)\kappa}$ satisfy the following eigenequation

$$\begin{pmatrix} C_{(2)}(n) \\ C(s) \\ \mathcal{C}(s') \end{pmatrix} \psi_m^{(\nu)\kappa} = \begin{pmatrix} \nu \\ m \\ \kappa \end{pmatrix} \psi_m^{(\nu)\kappa} ,$$
$$m = m_1, m_2, \ldots, m_{h_\nu} ,$$
$$\kappa = \kappa_1, \kappa_2, \ldots, \kappa_{\tau_\nu} , \quad N = \sum_\nu \tau_\nu h_\nu , \tag{4-76}$$

where $C(s)$ remains the set of $(n-2)$ 2–cycle class operators

$$C(s) = (C_{(2)}(n-1), C_{(2)}(n-2), \ldots C_{(2)}(2)) .$$

From (4-75) and (4-76) we obtain

$$\sum_{b=1}^{N} \left[\left\langle \varphi_a \left| \begin{matrix} C_{(2)}(n) \\ C(s) \\ \mathcal{C}(s') \end{matrix} \right| \varphi_b \right\rangle - \begin{pmatrix} \nu \\ m \\ \kappa \end{pmatrix} \delta_{ab} \right] u_{\nu m \kappa, b} = 0 . \tag{4-77}$$

The $\psi_m^{(\nu)\kappa}$ also satisfy orthogonality and completeness conditions

$$\langle \psi_m^{(\nu)\kappa} | \psi_{m'}^{(\nu')\kappa'} \rangle = \delta_{\nu\nu'} \delta_{mm'} \delta_{\kappa\kappa'} ,$$
$$\sum_{\nu m \kappa} |\psi_m^{(\nu)\kappa}\rangle \langle \psi_m^{(\nu)\kappa}| = 1 ,$$
$$\sum_{a=1}^{N} u^*_{\nu m \kappa, a} u_{\nu' m' \kappa', a} = \delta_{\nu\nu'} \delta_{mm'} \delta_{\kappa\kappa'} , \tag{4-78}$$
$$\sum_{\nu} \sum_{m=1}^{h_\nu} \sum_{\kappa=1}^{\tau_\nu} u^*_{\nu m \kappa, a} u_{\nu m \kappa, a'} = \delta_{aa'} .$$

Remark: Although (4-78) is similar in appearance to (3-216), (3-217) and (3-180), here the coefficients $u_{\nu m \kappa, a}$ are not related to the irreducible matrix elements $D^{(\nu)}_{m\kappa}(R_a)$. An example for finding $\psi_m^{(\nu)\kappa}$ is given in Sec. 4.9.

4.8.3. Projection operators and the quasi-standard basis

It is usually taken for granted (Bohr 1969 Appendix IC, Patterson 1976) that for the case of the non–regular rep one can still use the projection operator $P_m^{(\nu)k}$ to project out the standard basis of $\mathcal{S}_n$ out of the normal order state (4-70a).

$$\psi_m^{(\nu)k}(\omega) = P_m^{(\nu)k} |\omega\rangle , \quad P_m^{(\nu)k} = \sqrt{\frac{h_\nu}{g}} \sum_{a=1}^{n!} D^{(\nu)}_{mk}(p_a) p_a . \tag{4-79}$$

At first sight, it seems that using (3-169) and the relation $\bar{p} = \wp^{-1}$, we can easily "prove" that the basis (4-79) satisfies the following equations

$$\begin{pmatrix} C \\ C(s) \\ \mathcal{C}(s) \end{pmatrix} \psi_m^{(\nu)k}(\omega) = \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} \psi_m^{(\nu)k}(\omega) , \tag{4-80a}$$

$$\wp \psi_m^{(\nu)k}(\omega) = \sum_{k'} D^{(\nu)}_{k'k}(p) \psi_m^{(\nu)k'}(\omega) , \tag{4-80b}$$

whether or not the normal order state $|\omega\rangle$ contains identical state labels. We know from the previous subsection that among the eigenequations of $\mathcal{C}(s) = (\mathcal{C}(n-1), \mathcal{C}(n-2), \ldots, \mathcal{C}(2))$, only the eigenequations of $\mathcal{C}(s')$ [(4-73)] are meaningful. Thus among the quantum numbers $k = (\overline{\lambda}(n-n_1), \ldots, \overline{\lambda}(2))$, only the quantum numbers $\kappa = (\overline{\lambda}(n-n_l), \ldots, \overline{\lambda}(n_1+n_2), \overline{\lambda}(n_1))$ are true quantum numbers, the rest must be discarded. We also know that (4-80b) is false. What then is wrong with the "proof" of (4-80), and in what sense can (4-80) be regarded as correct? We say that (4-80) holds only formally. Namely, if each $\psi_m^{(\nu)k}$ is regarded as an independent basis vector no matter whether it is zero, or whether $\psi_m^{(\nu)k}$ and $\psi_m^{(\nu)k'}$ are linearly dependent and unnormalized. Therefore (4-80) only means that the operators $P_m^{(\nu)k}$ are the standard basis of the intrinsic permutation group $\overline{S}_n$ and does not imply in the least that the $\psi_m^{(\nu)k}$ are the standard basis of the state permutation group $\mathcal{S}_n$.

Let us now discuss how to correctly use and interpret the projection operator when it acts on the normal order state $|\omega\rangle$ with repeated state labels. In such cases $\psi_m^{(\nu)k}(\omega)$ of (4-79) is an unnormalized standard basis vector (ν, m) of S_n and a quasi-standard basis vector (ν, κ) of the state permutation group $\mathcal{S}_n$. Dropping the subscript m for clarity one has

$$\psi^{(\nu)k}(\omega) = P^{(\nu)k}|\omega\rangle = R^{(\nu)k}(\omega)\psi^{(\nu)\kappa}(\omega) \ , \tag{4-81a}$$

where we use $\psi^{(\nu)k}(\omega)(k$ include the false quantum numbers) and $\psi^{(\nu)\kappa}(\omega)(\kappa$ are the true quantum numbers) to denote an unnormalized and normalized basis vectors, respectively. $R^{(\nu)k}(\omega)$ is a normalization constant which can be calculated from

$$R^{(\nu)k}(\omega) = \left(\sqrt{\frac{n!}{h_\nu}}\langle\omega|P_k^{(\nu)k}|\omega\rangle\right)^{\frac{1}{2}} = \left[\left\langle\omega\middle|\sum_p D_{kk}^{(\nu)}(p)p\middle|\omega\right\rangle\right]^{\frac{1}{2}} = \left[\sum_p{}' D_{kk}^{(\nu)}(p)\right]^{\frac{1}{2}} \ . \tag{4-81b}$$

In deriving (4-81b), Eqs. (3-224) and (3-196) were used. The prime in the summation in (4-81b) indicates that the permutation p has to satisfy the condition $p|\omega\rangle = |\omega\rangle$. For example, one has

$$R^{[\nu]k}(\alpha\alpha\beta\gamma\gamma) = 1 + D_{kk}^{[\nu]}(12) + D_{kk}^{[\nu]}(45) + D_{kk}^{[\nu]}((12)(45)) \ . \tag{4-81c}$$

When all the state labels in $|\omega\rangle$ are distinct, the only operator which satisfies $p|\omega\rangle = |\omega\rangle$ is $p = e$ (identity), and thus $R^{(\nu)k}(\omega) = 1$. Then the quasi-standard basis is the standard basis. Table 4.8 gives normalization factors $R^{(\nu)k}(\omega)$ for S_2–S_4. A much better method for computing the normalization factor $R^{[\nu]k}(\omega)$ is given on p. 3453 of Chen & Chen (1983).

It is possible that several projection operators $P_m^{(\nu)k}$ in (4-81a) with different k give rise to the same quasi-standard basis $\psi^{(\nu)\kappa}$, since different k may lead to the same quantum number κ after deleting the false quantum numbers from k. For example, for the configuration $\alpha\beta^2\delta$, only $\mathcal{C}(4)$ and $\mathcal{C}(3)$ have definite action while $\mathcal{C}(2)$ is meaningless and the eigenvalue $\overline{\lambda}_2$ of $\mathcal{C}(2)$ should be deleted from k. Deleting the false quantum number $\overline{\lambda}_2 = \pm 1$ from k=(0,1) and $(0,-1)$ leads to the same quantum number $\kappa = 0$. From (4-81) and Table 4.8 we have

$$\psi^{(2)0,*}(\alpha\beta\beta\delta) = \sqrt{2}\psi^{(2)0,1}(\alpha\beta\beta\delta) = \sqrt{\frac{2}{3}}\psi^{(2)0,-1}(\alpha\beta\beta\delta) \ , \tag{4-82}$$

where $\psi^{(2)0,*}$ is a quasi-standard basis vector of $\mathcal{S}_4$, the asterisk at the position of $\bar{\lambda}_2$ indicating that it is not an eigenvector of $\mathcal{C}(2)$.

Table 4.8. Normalization factors $R^{(\nu)k}(\omega)$.

(ω) \ $[\nu]$ / m	[3]	[21]	
	1	1	2
$(\alpha\beta\beta)$	$\sqrt{2}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$

$(\bar{\omega})$ \ $[\nu]$ / m	[4]	[31]			[22]		[211]		
	1	1	2	3	1	2	1	2	3
$(\alpha\beta\gamma\gamma)$	$\sqrt{2}$	$\sqrt{\frac{2}{3}}$	$\sqrt{\frac{4}{3}}$	$\sqrt{2}$	$\sqrt{2}$			$\sqrt{\frac{2}{3}}$	$\sqrt{\frac{4}{3}}$
$(\alpha\alpha\beta\beta)$	2	$\sqrt{\frac{4}{3}}$	$\sqrt{\frac{8}{3}}$		2				
$(\alpha\beta\beta\beta)$	$\sqrt{6}$	$\sqrt{\frac{2}{3}}$	$\sqrt{\frac{4}{3}}$	2					

(ω) \ $[\nu]$ / m	[5]	[41]				[32]					[311]						[221]					[21^3]			
	1	1	2	3	4	1	2	3	4	5	1	2	3	4	5	6	1	2	3	4	5	1	2	3	4
$(\alpha\beta\gamma\delta\delta)$	$\sqrt{2}$	$\sqrt{\frac{3}{4}}$	$\sqrt{\frac{5}{4}}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	$\sqrt{\frac{3}{2}}$		$\sqrt{\frac{3}{4}}$	$\sqrt{\frac{3}{4}}$	$\sqrt{\frac{5}{4}}$	$\sqrt{\frac{5}{4}}$	$\sqrt{2}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{2}}$	$\sqrt{\frac{3}{2}}$				$\sqrt{\frac{3}{4}}$	$\sqrt{\frac{5}{4}}$
$(\alpha\alpha\beta\gamma\gamma)$	2	$\sqrt{\frac{3}{2}}$	$\sqrt{\frac{5}{2}}$	2		2	1		$\sqrt{3}$			$\sqrt{\frac{3}{2}}$		$\sqrt{\frac{5}{2}}$			1		$\sqrt{3}$						
$(\alpha\beta\beta\gamma\gamma)$	2	$\sqrt{\frac{3}{2}}$	$\sqrt{\frac{5}{2}}$	1	$\sqrt{3}$	2	$\frac{1}{2}$	$\sqrt{\frac{3}{4}}$	$\sqrt{\frac{3}{4}}$	$\frac{3}{2}$		$\sqrt{\frac{3}{8}}$	$\sqrt{\frac{9}{8}}$	$\sqrt{\frac{5}{8}}$	$\sqrt{\frac{15}{8}}$		$\frac{1}{2}$	$\sqrt{\frac{3}{4}}$	$\sqrt{\frac{3}{4}}$	$\frac{3}{2}$					
$(\alpha\beta\gamma\gamma\gamma)$	$\sqrt{6}$	1	$\sqrt{\frac{5}{3}}$	$\sqrt{\frac{10}{3}}$	$\sqrt{6}$	$\sqrt{\frac{2}{3}}$	$\sqrt{\frac{3}{4}}$		2				1		$\sqrt{\frac{5}{3}}$	$\sqrt{\frac{10}{3}}$									
$(\alpha\alpha\beta\beta\beta)$	$\sqrt{12}$	$\sqrt{2}$	$\sqrt{\frac{10}{3}}$	$\sqrt{\frac{20}{3}}$		$\sqrt{\frac{4}{3}}$	$\sqrt{\frac{8}{3}}$		$\sqrt{8}$																
$(\alpha\alpha\alpha\beta\beta)$	$\sqrt{12}$	$\sqrt{\frac{9}{2}}$	$\sqrt{\frac{15}{2}}$			$\sqrt{12}$																			
$(\alpha\beta\beta\beta\beta)$	$\sqrt{24}$	$\sqrt{\frac{3}{2}}$	$\sqrt{\frac{5}{2}}$	$\sqrt{5}$	$\sqrt{15}$																				

[1] A blank in the table means $R^{(\nu)k}(\omega)=0$.

[2] If all the single particle states in $|\omega\rangle$ are the same, then for the totally symmetric rep $[n]$, we have $R^{[n]}(\omega) = \sqrt{1/n!}$.

4.8.4. The labelling of the quasi-standard basis

In Sec. 4.7 we discussed the standard basis $\psi_m^{(\nu)k}(\omega_0)$ of S_n and $\overline{S}_n$, where $|\omega_0\rangle$ represents a normal order state with no repeated state labels. The state $\psi_m^{(\nu)k}(\omega)$ of (4-79), projected out of a normal order state $|\omega\rangle$ with repeated state labels, can be obtained from $\psi_m^{(\nu)k}(\omega_0)$ simply by letting $\omega_0 \to \omega$. For example

$$\psi_m^{(\nu)k}(\alpha\beta\beta\delta) = \psi_m^{(\nu)k}(\alpha\beta\gamma\delta)|_{\gamma=\beta} \,. \tag{4-83a}$$

This procedure is called *assimilation* . In Sec. 4.7.2, we used the Weyl tableau W_k to replace the quantum number k, that is, use $\psi_m^{(\nu)}(W_k)$ to denote $\psi_m^{(\nu)k}(\omega_0)$. Application of the assimilation procedure to $\psi_m^{(\nu)}(W_k)$ yields a Weyl table with repeated state labels. For instance, choosing $(\nu)k = (2),0,1$ and $(2),0,-1$, we can express (4-83a) in terms of the Weyl tableau

$$\psi_m^{(2)0,1}(\alpha\beta\beta\delta) = \psi_m^{[31]}\left(\begin{array}{|c|c|c|}\hline\alpha&\beta&\delta\\\hline\gamma\\\cline{1-1}\end{array}\right)\Big|_{\gamma=\beta} ,$$

$$\psi_m^{(2)0,-1}(\alpha\beta\beta\delta) = \psi_m^{[31]}\left(\begin{array}{|c|c|c|}\hline\alpha&\gamma&\delta\\\hline\beta\\\cline{1-1}\end{array}\right)\Big|_{\gamma=\beta} \,. \tag{4-83b}$$

It is thus seen that we can use Weyl tableaux with repeated state labels to denote the quasi-standard basis of the permutation group. Equation (4-82) can be rewritten as

$$\psi^{(2)0,*}(\alpha\beta\beta\delta) = \left|\begin{array}{|c|c|c|}\hline\alpha&\beta&\delta\\\hline\beta\\\cline{1-1}\end{array}\right\rangle = \sqrt{2}\psi\left(\begin{array}{|c|c|c|}\hline\alpha&\beta&\delta\\\hline\gamma\\\cline{1-1}\end{array}\right)\Big|_{\gamma=\beta} = \sqrt{\frac{2}{3}}\psi\left(\begin{array}{|c|c|c|}\hline\alpha&\gamma&\delta\\\hline\beta\\\cline{1-1}\end{array}\right)\Big|_{\gamma=\beta} .$$

It is easy to prove that if there are two identical state labels appearing in the same column of a Weyl tableau W_k, then the basis vector $|W_k\rangle = 0$. For example, we have

$$\left|\begin{array}{|c|c|c|}\hline\alpha&\gamma&\delta\\\hline\alpha\\\cline{1-1}\end{array}\right\rangle \propto \psi\left(\begin{array}{|c|c|c|}\hline\alpha&\gamma&\delta\\\hline\beta\\\cline{1-1}\end{array}\right)\Big|_{\beta=\alpha} = 0 \,.$$

Since the basis vector $\psi\left(\begin{array}{|c|c|c|}\hline\alpha&\gamma&\delta\\\hline\beta\\\cline{1-1}\end{array}\right)$ is anti-symmetric under the interchange of α and β, it vanishes when $\alpha = \beta$.

Now we give a general definition for the Weyl tableau.

A *Weyl tableau* is a Young diagram $[\nu]$ whose boxes are filled with the single particle states $m_1, m_2, \ldots, m_l$ under the restrictions that

(a) the same m value may not appear twice in any column,

(b) the m values must read in increasing order (first all m_1's, then m_2's, and so on) as we read from left to right in any row as well as from top to bottom in any column.

The labelling of the quasi-standard basis of the state permutation group in terms of the Weyl tableau is realized through the following scheme:

A Weyl tableau W_k filled with $m_1, \ldots, m_l$ is equivalent to l partitions $[\nu], [\nu^{l-1}], [\nu^{l-2}], \ldots, [\nu^2], [\nu^1]$. Here $[\nu^{l-1}], [\nu^{l-2}] \ldots$ are obtained by successively removing the boxes filled with m_l, $m_{l-1}, \ldots$ from the Weyl tableau W_k. The basis vector $|W_k\rangle$ is defined as the one belonging to the irreps $[\nu], [\nu^{l-1}], \ldots, [\nu^2], [\nu^1]$ of the state permutation group $\mathcal{S}_n, \mathcal{S}_{n-n_l}, \ldots, \mathcal{S}_{n_1+n_2}$ and $\mathcal{S}_{n_1}$. For example,

$$\begin{array}{|c|c|c|c|}\hline\alpha&\alpha&\beta&\gamma\\\hline\beta&\beta&\delta\\\cline{1-3}\gamma&\delta\\\cline{1-2}\end{array} \longrightarrow \begin{array}{|c|c|c|c|}\hline\alpha&\alpha&\beta&\gamma\\\hline\beta&\beta\\\cline{1-2}\gamma\\\cline{1-1}\end{array} \longrightarrow \begin{array}{|c|c|c|}\hline\alpha&\alpha&\beta\\\hline\beta&\beta\\\cline{1-2}\end{array} \longrightarrow \begin{array}{|c|c|}\hline\alpha&\alpha\\\hline\end{array}$$

$$S_9[432] \qquad S_7[421] \qquad S_5[32] \qquad S_2[2] \tag{4-84}$$

Finally we turn to the labelling question. We have the following four schemes for *labelling the quasi-standard basis* of $\mathcal{S}_n$.

1. By $\psi^{(\nu)k}(\omega)$: Here $|\omega\rangle$ is a normal order state.

Using Table 3.2-1, the l sets of eigenvalues $(\nu,k)=(\overline{\lambda}(n),\overline{\lambda}(n-n_l),\ldots,\overline{\lambda}(n_1))$ can be converted into l partitions, $[\nu]=[m_{1l}m_{2l}\ldots m_{ll}]$, $[\nu^{l-1}]=[m_{1l-1}m_{2l-1}\ldots m_{l-1l-1}],\ldots,[\nu^2]=[m_{12},m_{22}]$ and $[\nu^1]=[m_{11}]$. Thus it is equivalent to the second labelling scheme.

2. By the so-called *Gel'fand symbol* (see Sec. 7.4).

$$\begin{pmatrix}[\nu]\\(m)\end{pmatrix}=\begin{pmatrix} m_{1l}\ m_{2l}\ldots m_{ll}\\ m_{1l-1}\ldots m_{l-1,l-1}\\ \ldots\\ m_{12}m_{22}\\ m_{11}\end{pmatrix},\quad [\nu]=[m_{1l}\ldots m_{ll}]\,. \tag{4-85}$$

It belongs to the irreps $[\nu]=[m_{1l}\ldots m_{ll}],\ldots[m_{12}m_{22}]$ and $[m_{11}]$ of $\mathcal{S}_n,\ldots,\mathcal{S}_{n_1+n_2}$ and $\mathcal{S}_{n_1}$, respectively.

3. By a Weyl tableau $|W_k\rangle$.

4. By the Yamanouchi symbol and the normal order state, that is, by $\psi^{[\nu]r_k}(\omega)$.

Let us use the following three examples to illustrate these labelling schemes

(i) $|\omega\rangle=|\alpha\alpha\beta\gamma\gamma\rangle$

$$\psi^{(5),*,3,1}(\omega)=\left|\begin{pmatrix}4&1&0\\3&0\\2\end{pmatrix}\right\rangle=\left|\begin{array}{|c|c|c|c|}\hline\alpha&\alpha&\beta&\gamma\\\hline\gamma\\\cline{1-1}\end{array}\right\rangle\propto\psi^{[41]21111}(\omega)\propto\psi^{[41]12111}(\omega)\,.$$

This belongs to the irreps [41], [3] and [2] of $\mathcal{S}_5,\mathcal{S}_3$ and $\mathcal{S}_2$.

(ii) $|\omega\rangle=|\alpha\alpha\beta\beta\beta\rangle$

$$\psi^{(2),*,*,1}(\omega)=\left|\begin{pmatrix}3&2\\2\end{pmatrix}\right\rangle=\left|\begin{array}{|c|c|c|}\hline\alpha&\alpha&\beta\\\hline\beta&\beta\\\cline{1-2}\end{array}\right\rangle\propto\psi^{[32]22111}(\omega)\propto\psi^{[32]21211}(\omega)\propto\psi^{[32]12211}(\omega)$$

This belongs to the irreps [32] and [2] of $\mathcal{S}_5$ and $\mathcal{S}_2$.

(iii) $|\omega\rangle=|\alpha\beta\beta\beta\gamma\gamma\rangle$

$$\psi^{(3,4),*,2,*,*}(\omega)=\left|\begin{pmatrix}4&1&1\\3&1\\1\end{pmatrix}\right\rangle=\left|\begin{array}{|c|c|c|c|}\hline\alpha&\beta&\beta&\gamma\\\hline\beta\\\cline{1-1}\gamma\\\cline{1-1}\end{array}\right\rangle,$$

$$\psi^{(3,-8),*,2,*,*}(\omega)=\left|\begin{pmatrix}3&3&0\\3&1\\1\end{pmatrix}\right\rangle=\left|\begin{array}{|c|c|c|}\hline\alpha&\beta&\beta\\\hline\beta&\gamma&\gamma\\\cline{1-3}\end{array}\right\rangle.$$

Here (3, 4) and (3, −8) are the eigenvalues of the CSCO-I, $\mathcal{C}=(\mathcal{C}_{(2)}(6),\mathcal{C}_{(3)}(6))$. The eigenvalue 3 of $\mathcal{C}_{(2)}(6)$ is no longer sufficient to specify the irrep $[\nu]$, since the group chain $\mathcal{S}_6\supset\mathcal{S}_4\supset\mathcal{S}_1$ is broken. This is why we should understand the operators $C(j)(j=n,n-n_l,\ldots,n_1+n_2,n_1)$ in (4-73a) as the CSCO-I of $\mathcal{S}_j$ instead of the 2-cycle class operator of $\mathcal{S}_j$.

It is seen that the first three labelling schemes are in one–to–one correspondence

$$\psi^{(\nu)\kappa}(\omega)=\left|\begin{pmatrix}[\nu]\\m\end{pmatrix}\right\rangle=|W_\kappa^{[\nu]}\rangle\,, \tag{4-86}$$

while the labelling with the Yamanouchi symbol r_k is not unique, as there may be several r_k's corresponding to the same state. If there are no identical state labels in $|\omega\rangle$, that is, for the standard basis of $\mathcal{S}_n$, the four labelling schemes will all be in one–to–one correspondence.

We used the flight route of Fig. 4.5-3 to represent a Yamanouchi basis vector of S_n or $\mathcal{S}_n$. The flight route is labelled by the names $\lambda_n,\lambda_{n-1},\ldots,\lambda_2$ for the $n-1$ 'airports' passed through.

We can also use a flight route to represent a quasi-standard basis vector of $\mathcal{S}_n$. But now it is an 'express flight route' which only passes $l < n$ 'airports'. The express flight route is labelled by the names $\overline{\lambda}(n), \overline{\lambda}(n-n_l), \ldots, \overline{\lambda}(n_1)$ of the l 'airports.' Obviously, the total number τ_ν of possible express routes is less than the number h_ν of all possible local routes. We use the irrep $\nu = 5$ (or $[\nu] = [41]$) of $\mathcal{S}_5$ as an example to illustrate the difference between these two cases.

configuration $\alpha\beta\gamma\delta\varepsilon$

Irrep (5) has $h_\nu = 4$ standard basis vectors

$$\left|\begin{array}{|c|c|c|c|}\hline\alpha&\beta&\gamma&\delta\\\hline\varepsilon\\\cline{1-1}\end{array}\right\rangle = \psi^{(5),6,3,1}(\alpha\beta\gamma\delta\varepsilon)$$

$$\left|\begin{array}{|c|c|c|c|}\hline\alpha&\beta&\gamma&\varepsilon\\\hline\delta\\\cline{1-1}\end{array}\right\rangle = \psi^{(5),2,3,1}(\alpha\beta\gamma\delta\varepsilon)$$

$$\left|\begin{array}{|c|c|c|c|}\hline\alpha&\beta&\delta&\varepsilon\\\hline\gamma\\\cline{1-1}\end{array}\right\rangle = \psi^{(5),2,0,1}(\alpha\beta\gamma\delta\varepsilon)$$

$$\left|\begin{array}{|c|c|c|c|}\hline\alpha&\gamma&\delta&\varepsilon\\\hline\beta\\\cline{1-1}\end{array}\right\rangle = \psi^{(5),2,0,-1}(\alpha\beta\gamma\delta\varepsilon)$$

Starting from the airport (5) there are $h_\nu = 4$ flight routes: (5,6,3,1), (5,2,3,1), (5,2,0,1), and (5,2,0,−1).

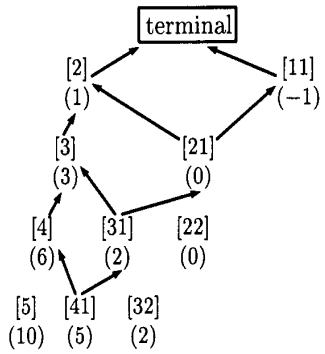


Fig. 4.8-1a. The standard basis of $\mathcal{S}_5$.

configuration $(\alpha)^2\beta(\gamma)^2$

Irrep (5) has $\tau_\nu = 2$ quasi-standard basis vectors

$$\left|\begin{array}{|c|c|c|c|}\hline\alpha&\alpha&\beta&\gamma\\\hline\gamma\\\cline{1-1}\end{array}\right\rangle = \psi^{(5),*,3,1}(\alpha\alpha\beta\gamma\gamma)$$

$$\left|\begin{array}{|c|c|c|c|}\hline\alpha&\alpha&\gamma&\gamma\\\hline\beta\\\cline{1-1}\end{array}\right\rangle = \psi^{(5),*,0,1}(\alpha\alpha\beta\gamma\gamma)$$

Starting from the airport (5), there are $\tau_\nu = 2$ express flight routes: (5, *, 3, 1) and (5, *, 0, 1).

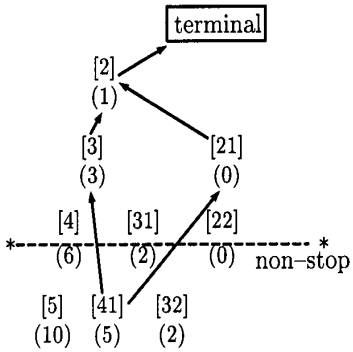


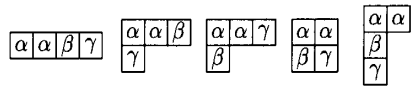
Fig. 4.8-1b. The quasi-standard basis of $\mathcal{S}_5$.

4.9. The EFM for the Yamanouchi Basis (II)

In this section we will use the Weyl tableaux and the intrinsic quantum number to simplify the calculation of the standard basis of S_n. The basis calculated in this way is also a quasi-standard basis of $\mathcal{S}_n$. The first three steps and the fifth step are identical to those given in Sec. 4.6. Only the fourth step should be modified into:

4a. For the configuration $(\alpha)^{n_1}(\beta)^{n_2}\ldots$ of an n-particle system, write out all possible Weyl tableaux. The number of Weyl tableaux corresponding to a given partition $[\nu]$ gives the multiplicity τ_ν. According to the relation between the Young diagrams $[\nu]$ and the eigenvalues λ_n, Eq. (4-3a) or Fig. 4.5-3, we then know the eigenvalue λ_n and its degeneracy τ_ν. Thus the problem of finding the roots of the expectation equation is avoided.

Example: The configuration $\alpha^2\beta\gamma$ has the following Weyl tableaux:



(4-87a)

Therefore $\tau_{[4]} = \tau_{[22]} = \tau_{[211]} = 1$ and $\tau_{[31]} = 2$. According to Fig. 4.5-3, we know that the corresponding eigenvalues are $\lambda_4 = 6,\ 0,\ -2$ (single roots) and $\lambda_4 = 2$ (double root).

4b. For the $\tau_\nu = 1$ case, the eigenequations of $(C, C(s))$ are sufficient to fix the solution completely. For the $\tau_\nu > 1$ case, we also need the eigenequations of $\mathcal{C}(s')$ to fix the solutions. From the Weyl tableaux determined in step (4a), we know the corresponding eigenvalues κ of $\mathcal{C}(s')$ without solving the expectation equation. On substituting the eigenvalues into (4-77), we can obtain the solutions $u_{\nu m\kappa,a}$.

As an example, we again take the configuration $\alpha^2\beta\gamma$ discussed in Sec. 4.6. For this configuration, the elements of $\mathcal{S}_2$ are equivalent to the identity element, and the CSCO of $\mathcal{S}_3$ is meaningful. In Sec. 4.6, we arbitrarily chose two independent solutions in (4-49). Now we can employ the eigenequation of $\mathcal{C}(s') = \mathcal{C}(3)$ to fix the solutions completely. In (4-48) there are two independent variables which can be chosen as u_4 and u_2. Applying $\mathcal{C}(3)$ to $\varphi_4 = |\gamma\alpha\beta\alpha\rangle$, we obtain

$$\begin{aligned}\mathcal{C}(3)\varphi_4 &= \mathcal{C}(3)|\gamma\alpha\beta\alpha\rangle = (\wp_{12} + \wp_{23} + \wp_{13})|i_4 i_1 i_3 i_2\rangle \\ &= |\gamma\alpha\beta\alpha\rangle + |\gamma\alpha\alpha\beta\rangle + |\gamma\beta\alpha\alpha\rangle = \varphi_4 + \varphi_7 + \varphi_{12}\ .\end{aligned} \tag{4-87b}$$

Using (3-75b) we get an equation involving the variable u_4,

$$u_4 + u_7 + u_{12} = \overline{\lambda}_3 u_4.$$

Using (4-43) and (4-48a), this becomes

$$3u_4 + u_{10} = \overline{\lambda}_3 u_4. \tag{4-87c}$$

The Weyl tableau $\begin{array}{|c|c|c|}\hline\alpha&\alpha&\beta\\\hline\gamma\\\cline{1-1}\end{array}$ in (4-87a) corresponds to $\overline{\lambda}_3 = 3$. Substituting it into (4-87c), we get a solution: $u_{10} = 0, u_4 = 1$. This is just the first solution (4-49a) we have chosen. Another Weyl tableau $\begin{array}{|c|c|c|}\hline\alpha&\alpha&\gamma\\\hline\beta\\\cline{1-1}\end{array}$ in (4-87a) corresponds to $\overline{\lambda}_3 = 0$. The corresponding solution of (4-87c) is: $u_4 = -1$ and $u_{10} = 3$. This is just the solution (4-49c).

The third and fourth steps in Sec. 4.6 can also be modified into the following steps: Associate with each permissible Weyl tableau W_κ a Young tableau Y_m. From Y_m and W_κ write down the corresponding eigenvalues (ν, m, κ). Substituting the eigenvalues into (4-76), we can find the eigenfunction $\psi_m^{(\nu)\kappa} = |Y_m, W_\kappa\rangle$. Then use (4-36) to get the other components.

Ex. 4.4. Find the standard basis of $\mathcal{S}_4$ and the quasi-standard basis of $\mathcal{S}_4$ for the configuration $\alpha\beta\gamma^2$ (the answer is given in Table 4.9).

Table 4.9. The standard basis[1] of S_4 and quasi-standard basis of S_4 for the configuration $(\alpha)(\beta)(\gamma)^2$.

$\lambda_4\lambda_3\lambda_2$	$\bar{\lambda}_2$	Young tableau	Weyl tableau	$\lvert\alpha\beta\gamma\gamma\rangle$	$\lvert\beta\alpha\gamma\gamma\rangle$	$\lvert\gamma\alpha\beta\gamma\rangle$	$\lvert\gamma\beta\alpha\gamma\rangle$	$\lvert\beta\gamma\alpha\gamma\rangle$	$\lvert\alpha\gamma\beta\gamma\rangle$	$\lvert\gamma\alpha\gamma\beta\rangle$	$\lvert\gamma\beta\gamma\alpha\rangle$	$\lvert\gamma\gamma\beta\alpha\rangle$	$\lvert\gamma\gamma\alpha\beta\rangle$	$\lvert\beta\gamma\gamma\alpha\rangle$	$\lvert\alpha\gamma\gamma\beta\rangle$
6, 3, 1	1	1234	$\alpha\beta\gamma\gamma$	$\boxed{\sqrt{\frac{1}{12}}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$
2, 3, 1	1	123 4		$\boxed{\sqrt{\frac{1}{12}}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$\sqrt{\frac{1}{12}}$	$-\sqrt{\frac{1}{12}}$	$-\sqrt{\frac{1}{12}}$	$-\sqrt{\frac{1}{12}}$	$-\sqrt{\frac{1}{12}}$	$-\sqrt{\frac{1}{12}}$	$-\sqrt{\frac{1}{12}}$
2, 0, 1	1	124 3	$\alpha\beta\gamma$ γ	$\boxed{\sqrt{\frac{1}{6}}}$	$\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{24}}$	$-\sqrt{\frac{1}{24}}$	$-\sqrt{\frac{1}{24}}$	$-\sqrt{\frac{1}{24}}$	$\sqrt{\frac{1}{24}}$	$\sqrt{\frac{1}{24}}$	$-\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{24}}$	$\sqrt{\frac{1}{24}}$
2, 0, −1	1	134 2				$-\sqrt{\frac{1}{8}}$	$-\sqrt{\frac{1}{8}}$	$\sqrt{\frac{1}{8}}$	$\boxed{\sqrt{\frac{1}{8}}}$	$-\sqrt{\frac{1}{8}}$	$-\sqrt{\frac{1}{8}}$			$\sqrt{\frac{1}{8}}$	$\sqrt{\frac{1}{8}}$
2, 3, 1	−1	123 4								$\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{6}}$	$\boxed{\sqrt{\frac{1}{6}}}$
2, 0, 1	−1	124 3	$\alpha\gamma\gamma$ β			$\sqrt{\frac{3}{16}}$	$-\sqrt{\frac{3}{16}}$	$-\sqrt{\frac{3}{16}}$	$\boxed{\sqrt{\frac{3}{16}}}$	$\sqrt{\frac{1}{48}}$	$-\sqrt{\frac{1}{48}}$	$\sqrt{\frac{1}{12}}$	$-\sqrt{\frac{1}{12}}$	$-\sqrt{\frac{1}{48}}$	$\sqrt{\frac{1}{48}}$
2, 0, −1	−1	134 2		$\boxed{\frac{1}{2}}$	$-\frac{1}{2}$	$-\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$			$-\frac{1}{4}$	$\frac{1}{4}$
−2, 0, 1	−1	12 3 4				$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\boxed{\frac{1}{4}}$	$-\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{4}$	$-\frac{1}{4}$
−2, 0, −1	−1	13 2 4	$\alpha\gamma$ β γ	$\boxed{\sqrt{\frac{1}{12}}}$	$-\sqrt{\frac{1}{12}}$	$-\sqrt{\frac{1}{48}}$	$\sqrt{\frac{1}{48}}$	$-\sqrt{\frac{1}{48}}$	$\sqrt{\frac{1}{48}}$	$\sqrt{\frac{3}{16}}$	$-\sqrt{\frac{3}{16}}$			$\sqrt{\frac{3}{16}}$	$-\sqrt{\frac{3}{16}}$
−2, −3, −1	−1	14 2 3		$\boxed{\sqrt{\frac{1}{6}}}$	$-\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{6}}$						
0, 0, 1	1	12 34	$\alpha\beta$ $\gamma\gamma$	$\boxed{\sqrt{\frac{1}{6}}}$	$\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{24}}$	$-\sqrt{\frac{1}{24}}$	$-\sqrt{\frac{1}{24}}$	$-\sqrt{\frac{1}{24}}$	$-\sqrt{\frac{1}{24}}$	$-\sqrt{\frac{1}{24}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{24}}$	$-\sqrt{\frac{1}{24}}$
0, 0, −1	1	13 24				$-\sqrt{\frac{1}{8}}$	$-\sqrt{\frac{1}{8}}$	$\sqrt{\frac{1}{8}}$	$\boxed{\sqrt{\frac{1}{8}}}$	$\sqrt{\frac{1}{8}}$	$\sqrt{\frac{1}{8}}$			$-\sqrt{\frac{1}{8}}$	$-\sqrt{\frac{1}{8}}$

[1] The framed entries are the principle terms [see (4-60)].

4.10. The Inner Product and the CG Series of Permutation Groups

The state of a microscopic particle is described by a wave function $\psi(q)$, with q representing all the coordinates. For example, for an electron, q represents the orbital and spin coordinates; for a nucleon, q includes the orbital, spin and isospin coordinates; for a quark, q denotes the orbital, spin, flavor and color coordinates. In treating the permutation symmetry of an n–particle system, we usually first consider the symmetry for the individual degrees of freedom and then treat the symmetry governing the full problem with all degrees of freedom included. For example, we divide the coordinate q into two parts

$$q = (x, \xi) ,$$

where x and ξ may represent the orbital and spin–isospin coordinates respectively, or represent spin and isospin coordinates respectively, and so on. We now have three realizations of the permutation group S_n, they are

permutation group,	permutation operator,	permutation object,	irreducible basis
$S_n(x)$	${}^{x}p$	x	$\varphi_{m_1}^{(\nu_1)}(x)$
$S_n(\xi)$	${}^{\xi}p$	ξ	$\psi_{m_2}^{(\nu_2)}(\xi)$
$S_n(q)$	${}^{q}p \equiv p$	$q = (x, \xi)$	$\Psi_m^{(\nu)\tau}(q)$

According to the definition, we have

$$[{}^{x}p, {}^{\xi}p] = 0 , \quad p = {}^{x}p\,{}^{\xi}p .$$

The permutation group $S_n(q)$ is called the *inner-product* of $S_n(x)$ and $S_n(\xi)$. Suppose $\varphi_{m_1}^{\nu_1}(x)$ and $\psi_{m_2}^{\nu_2}(\xi)$ are the irreducible basis of $S_n(x)$ and $S_n(\xi)$, respectively. The reduction of the Kronecker product rep with the basis $\varphi_{m_1}^{\nu_1}(x)\psi_{m_2}^{\nu_2}(\xi)$ into the irreps of $S_n(q)$ is called the *inner-product reduction* of the permutation group. In other words, the inner product reduction deals with the problem of how to linearly combine the products of wave functions with definite permutation symmetries in each individual degree of freedom into a wave function with a definite permutation symmetry in the overall degrees of freedom.

The CG series of the permutation group is designated

$$[\nu_1] \times [\nu_2] = \sum_{\nu} (\nu_1 \nu_2 \nu)[\nu] .$$

The multiplicity $(\nu_1\nu_2\nu)$ is determined by (3-274). Noting that all the primitive characters of the permutation group are real, (3-274) becomes

$$(\nu_1\nu_2\nu) = \frac{1}{g}\sum_i g_i \chi_i^{(\nu_1)}\chi_i^{(\nu_2)}\chi_i^{(\nu)} , \tag{4-88}$$

and we also know that $(\nu_1\nu_2\nu)$ satisfies the relation (3-276).

Using $\chi_i^{(\tilde{\nu})} = \delta_i \chi_i^{(\nu)}$, from (4-5), in (4-88) one finds

$$(\nu_1\nu_2\nu) = (\tilde{\nu}_1\tilde{\nu}_2\nu) = (\nu_1\tilde{\nu}_2\tilde{\nu}) = (\tilde{\nu}_1\nu_2\tilde{\nu}) . \tag{4-89}$$

Since $\chi_i^{[n]} = 1$ and $\chi_i^{[1^n]} = \delta_i$, we know immediately that

$$[\nu] \times [n] = [\nu], \quad [\nu] \times [1^n] = [\tilde{\nu}] . \tag{4-90}$$

From the simple characters of the permutation group and (4-88), one can calculate the CG series of the permutation group. Tables of the CG series for the permutation group up to S_8 are given by Itzykson (1966). Table 4.10 gives the CG series of S_3–S_5.

Table 4.10. CG series of S_3-S_5*.

(*a*) S_3 group

	[3]	[21]	[1³]
[21]×[21]	1	1	1

(*b*) S_4 group

	[4]	[31]	[22]	[211]	[1⁴]	
[31]×[31]	1	1	1	1		[31]×[211], [211]×[31]
[31]×[22]		1		1		[31]×[22], [211]×[22]
[22]×[22]	1		1		1	[22]×[22], [22]×[22]
	[1⁴]	[211]	[22]	[31]	[4]	

(*c*) S_5 group

	[5]	[41]	[32]	[311]	[221]	[21³]	[1⁵]	
[41]×[41]	1	1	1	1				[41]×[21³], [21³]×[41]
[41]×[32]		1	1	1	1			[41]×[2²1], [21³]×[32]
[41]×[311]		1	1	1	1	1		[41]×[311], [21³]×[311]
[32]×[32]	1	1	1	1	1	1		[32]×[2²1], [221]×[32]
[32]×[311]		1	1	2	1	1		[32]×[311], [221]×[311]
[311]×[311]	1	1	2	1	2	1	1	[311]×[311], [311]×[311]
	[1⁵]	[21³]	[2²1]	[311]	[32]	[41]	[5]	

*The left(right) heading matches the top(bottom) heading.

Ex. 4.5. Use (4-88) and the characters of S_4 in Ex. 3.16 to confirm the CG series for S_4 given in Table 4-10.

4.11. Calculation of the CG Coefficients of Permutation Groups

We use $|m_1 m_2\rangle$ (or $(m_1 m_2)$, as shown in Table 4.13) to denote the product basis

$$|m_1 m_2\rangle = \varphi_{m_1}^{[\nu_1]}(x)\psi_{m_2}^{[\nu_2]}(\xi) = |Y_{m_1}^{[\nu_1]} Y_{m_2}^{[\nu_2]}\rangle \ . \tag{4-91}$$

Employing the CG coefficients $C_{\nu_1 m_1,\nu_2 m_2}^{[\nu]\tau,m}$, the product basis can be linearly combined into the irreducible basis $\Psi_m^{[\nu]\tau}(q)$ of the group $S_n(q)$

$$\Psi_m^{[\nu]\tau}(q) = \sum_{m_1 m_2} C_{\nu_1 m_1,\nu_2 m_2}^{[\nu]\tau,m} \varphi_{m_1}^{(\nu_1)}(x)\psi_{m_2}^{(\nu_2)}(\xi), \quad \tau = 1,2,\ldots(\nu_1\nu_2\nu) \ , \tag{4-92a}$$

where τ is the multiplicity label. From (4-91) and (4-92a), we obtain

$$C_{\nu_1 m_1,\nu_2 m_2}^{[\nu]\tau,m} = \langle Y_m^{[\nu]\tau}(q)|Y_{m_1}^{[\nu_1]} Y_{m_2}^{[\nu_2]}\rangle \ . \tag{4-92b}$$

The CG coefficients of the permutation group are quite useful (see Secs. 7.9 and 7.16). Hamermesh (1962) has calculated the CG coefficients for the product [311]× [311] by a recursive method. Vanagas (1972) gave some algebraic formulas for the CG coefficients in a few special cases. Schindler (1977) calculated the CG coefficients of S_n for $n \leq 6$ using the tensor product decomposition method.

The problems of obtaining the CG coefficients and obtaining the CG series can be solved simultaneously by the EFM. From (3-293) and (4-28c) we obtained the eigenequation satisfied by the CG coefficients of S_n,

$$\begin{gathered} \sum_{m_1 m_2} \left[\langle m_1' m_2'|C(f)|m_1 m_2\rangle - \lambda_f \delta_{m_1' m_1}\delta_{m_2' m_2}\right] C_{\nu_1 m_1,\nu_2 m_2}^{[\nu]\tau,m} = 0 \ , \\ f = n, n-1, \ldots, 2, \quad \tau = 1,2,\ldots,(\nu_1\nu_2\nu) \ , \\ (\nu, m) = (\lambda_n, \lambda_{n-1}, \ldots, \lambda_2) \ . \end{gathered} \tag{4-93}$$

The matrix elements of the 2–cycle class operator can be calculated recursively by using

$$\langle m_1' m_2' | C(f) | m_1 m_2 \rangle = \langle m_1' m_2' | C(f-1) | m_1 m_2 \rangle + \sum_{i=1}^{f-1} D^{(\nu_1)}_{m_1' m_1}(if) D^{(\nu_2)}_{m_2' m_2}(if) \ . \tag{4-94}$$

Let $N = h_1 h_2, h_i$ being the dimension of the irrep $[\nu_i]$ of S_f. The representative of $C(f)$ in the product (or uncoupled) rep is a $N \times N$ matrix given by

$$\mathbf{C}(f) = |\langle m_1' m_2' | C(f) | m_1 m_2 \rangle|_1^N \ . \tag{4-95}$$

The unitary transformation matrix which brings the $n-1$ matrices $\mathbf{C}(n), \mathbf{C}(n-1), \ldots, \mathbf{C}(2)$ simultaneously into diagonal form gives the CG coefficients.

It can be shown that the matrix elements of $\mathbf{C}(f)$ have the following properties:

1. $\mathbf{C}(f)$ is a real and symmetric matrix, that is,

$$\begin{aligned} \langle m_1' m_2' | C(f) | m_1 m_2 \rangle &= \langle m_1 m_2 | C(f) | m_1' m_2' \rangle \\ &= \langle m_1 m_2' | C(f) | m_1' m_2 \rangle = \langle m_1' m_2 | C(f) | m_1 m_2' \rangle \ . \end{aligned} \tag{4-96}$$

2. From (4-67), we have

$$\langle \tilde{m}_1' \tilde{m}_2' | C(f) | \tilde{m}_1 \tilde{m}_2 \rangle = \Lambda^{\nu_1}_{m_1'} \Lambda^{\nu_2}_{m_2'} \Lambda^{\nu_1}_{m_1} \Lambda^{\nu_2}_{m_2} \langle m_1' m_2' | C(f) | m_1 m_2 \rangle \ . \tag{4-97}$$

From (4-97) we can derive a symmetry relation for the CG coefficients. Rewriting (4-93) in the form

$$\sum_{\tilde{m}_1 \tilde{m}_2} \langle \tilde{m}_1' \tilde{m}_2' | C(f) | \tilde{m}_1 \tilde{m}_2 \rangle C^{[\nu]\tau, m}_{\tilde{\nu}_1 \tilde{m}_1, \tilde{\nu}_2 \tilde{m}_2} = \lambda_f C^{[\nu]\tau, m}_{\tilde{\nu}_1 \tilde{m}_1', \tilde{\nu}_2 \tilde{m}_2'} \ , \tag{4-98}$$

and inserting (4-97) into (4-98), we have

$$\sum_{m_1 m_2} \langle m_1' m_2' | C(f) | m_1 m_2 \rangle \Lambda^{\nu_1}_{m_1} \Lambda^{\nu_2}_{m_2} C^{[\nu]\tau, m}_{\tilde{\nu}_1 \tilde{m}_1, \tilde{\nu}_2 \tilde{m}_2} = \lambda_f \Lambda^{\nu_1}_{m_1'} \Lambda^{\nu_2}_{m_2'} C^{[\nu]\tau, m}_{\tilde{\nu}_1 \tilde{m}_1', \tilde{\nu}_2 \tilde{m}_2'} \ . \tag{4-99}$$

Comparing (4-93) with (4-99), we see that

$$\Lambda^{\nu_1}_{m_1} \Lambda^{\nu_2}_{m_2} C^{[\nu]\tau, m}_{\tilde{\nu}_1 \tilde{m}_1, \tilde{\nu}_2 \tilde{m}_2} = \eta^{\nu_\tau}_m \sum_{\tau'} a_{\tau\tau'} C^{[\nu]\tau', m}_{\nu_1 m_1, \nu_2 m_2} \ . \tag{4-100a}$$

Therefore

$$C^{[\nu]\tau, m}_{\tilde{\nu}_1 \tilde{m}_1, \tilde{\nu}_2 \tilde{m}_2} = \eta^{\nu_\tau}_m \Lambda^{\nu_1}_{m_1} \Lambda^{\nu_2}_{m_2} \sum_{\tau'} a_{\tau\tau'} C^{[\nu]\tau' m}_{\nu_1 m_1, \nu_2 m_2} \ . \tag{4-100b}$$

If $[\tilde{\nu}_1] \neq [\nu_1]$, or $[\tilde{\nu}_2] \neq [\nu_2]$, we can always choose the CG coefficients so that they satisfy the following symmetry

$$C^{[\nu]\tau, m}_{\tilde{\nu}_1 \tilde{m}_1, \tilde{\nu}_2 \tilde{m}_2} = \eta^{\nu_\tau}_m \Lambda^{\nu_1}_{m_1} \Lambda^{\nu_2}_{m_2} C^{[\nu]\tau, m}_{\nu_1 m_1, \nu_2 m_2} \ . \tag{4-101}$$

We will now prove that the phase factor $\eta^{\nu_\tau}_m$ is independent of m and depends only on ν_1, ν_2, ν and τ, that is,

$$\eta^{\nu_\tau}_m = \varepsilon_2(\nu_1 \nu_2 \nu_\tau) \equiv \varepsilon_2 = \pm 1 \ . \tag{4-102}$$

Using (4-92a), (4-101), (4-97) and (3-287) we have

$$\begin{aligned} D^{(\nu)}_{mm'}(p) \equiv \langle \Psi^{[\nu]\tau}_m | p | \Psi^{[\nu]\tau}_{m'} \rangle^* &= \sum_{\tilde{m}_1 \tilde{m}_2 \tilde{m}_1' \tilde{m}_2'} C^{[\nu]\tau, m}_{\tilde{\nu}_1 \tilde{m}_1, \tilde{\nu}_2 \tilde{m}_2} C^{[\nu]\tau, m'}_{\tilde{\nu}_1 \tilde{m}_1', \tilde{\nu}_2 \tilde{m}_2'} \langle \tilde{m}_1 \tilde{m}_2 | p | \tilde{m}_1' \tilde{m}_2' \rangle \\ &= \eta^{\nu_\tau}_m \eta^{\nu_\tau}_{m'} \sum_{m_1 m_2 m_1' m_2'} C^{[\nu]\tau, m}_{\nu_1 m_1, \nu_2 m_2} C^{[\nu]\tau, m'}_{\nu_1 m_1', \nu_2 m_2'} D^{(\nu_1)}_{m_1 m_1'}(p) D^{(\nu_2)}_{m_2 m_2'}(p) \\ &= \eta^{\nu_\tau}_m \eta^{\nu_\tau}_{m'} D^{(\nu)}_{mm'}(p) \ . \end{aligned}$$

Therefore

$$\eta_m^{\nu_\tau}\eta_{m'}^{\nu_\tau} = 1 \,, \tag{4-103}$$

for any m and m'. Consequently $\eta_m^{\nu_\tau}$ is independent of m.

From (4-102) and (4-101), we finally arrive at an important relation:

$$C^{[\nu]\tau,m}_{\tilde{\nu}_1\tilde{m}_1,\tilde{\nu}_2\tilde{m}_2} = \varepsilon_4(\nu_1\nu_2\nu_\tau)\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2}C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2} \,. \tag{4-104}$$

The phase factor $\varepsilon_4 = \pm 1$ is dictated by the overall phase convention (see (4-122a)).

By virtue of relation (4-104), we only need to calculate the CG coefficients for those $[\nu_1]$ and $[\nu_2]$ whose row length is greater than or equal to the column length.

If both $[\nu_1]$ and $[\nu_2]$ are self-conjugate, the following situations should be discussed separately.

(a). $(\nu_1\nu_2\nu) = 1$. In these cases the relation (4-104) holds automatically.

(b). $(\nu_1\nu_2\nu) = 2$. Two situations appear here. (i) Two sets of the CG coefficients $C^{[\nu]_{\alpha,m}}_{\nu_1 m_1,\nu_2 m_2}$ and $C^{[\nu]\beta,m}_{\nu_1 m_1,\nu_2 m_2}$ are both "symmetric" (the phase factor $\varepsilon_4 = 1$ for $\tau = \alpha,\beta$) or both "anti-symmetric" ($\varepsilon_4 = -1$ for $\tau = \alpha,\beta$). In such an instance, the CG coefficients calculated fulfill (4-104) automatically. (ii) Two sets of the CG coefficients contain both the "symmetric" and "anti-symmetric" components. In this case they can be recombined linearly into a "symmetric" and an "anti-symmetric" CG coefficient associated with $\varepsilon_4 = 1$ and -1, respectively.

(c). $(\nu_1\nu_2\nu) \geq 3$. See Gao & Chen (1985).

3. From $C(2) = {}^xC(2){}^\xi C(2)$, and

$${}^xC(2)\varphi^{[\nu_1]}_{m_1}(x) = \lambda_2^{(1)}\varphi^{[\nu_1]}_{m_1}(x) \,, \quad {}^\xi C(2)\psi^{[\nu_2]}_{m_2}(\xi) = \lambda_2^{(2)}\psi^{[\nu_2]}_{m_2}(\xi) \,,$$
$$\lambda_2^{(i)} = \pm 1 \,, \quad i = 1,2 \,,$$

we have

$$\begin{aligned} C(2)|m_1m_2\rangle &= \lambda_2|m_1m_2\rangle \,, \\ \lambda_2 &= \lambda_2^{(1)}\lambda_2^{(2)} \,. \end{aligned} \tag{4-105}$$

Thus $\mathbf{C}(2)$ is already diagonalized in the uncoupled representation. We only need to diagonalize the $n-2$ matrices $\mathbf{C}(3)$, $\mathbf{C}(4)$, $\ldots$, $\mathbf{C}(n)$.

4. From $[C(f), C(2)] = 0$, we have

$$\langle m_1'm_2'|C(f)C(2)|m_1m_2\rangle = \langle m_1'm_2'|C(2)C(f)|m_1m_2\rangle \,.$$

Therefore

$$\begin{aligned} \lambda_2\langle m_1'm_2'|C(f)|m_1m_2\rangle &= \lambda_2'\langle m_1'm_2'|C(f)|m_1m_2\rangle \,, \\ \langle m_1'm_2'|C(f)|m_1m_2\rangle &= 0, \quad \text{for} \quad \lambda_2 \neq \lambda_2' \,. \end{aligned} \tag{4-106}$$

Equation (4-106) tells us that there is no coupling between the basis vectors with $\lambda_2 = 1$ (denoted as $|m_1m_2\rangle_+$) and those with $\lambda_2 = -1$ (denoted as $|m_1m_2\rangle_-$). By appropriate ordering of $|m_1m_2\rangle$, the matrices $\mathbf{C}(f)$ becomes block-diagonalized, that is

$$\mathbf{C}(f) = \left(\begin{array}{c|c} \mathbf{C}^{(+)}(f) & 0 \\ \hline 0 & \mathbf{C}^{(-)}(f) \end{array}\right) \,, \quad f = 3,4,\ldots,n \,, \tag{4-107}$$

$$\mathbf{C}^{(\pm)}(f) = \|\langle m_1'm_2'|C(f)|m_1m_2\rangle_\pm\|_1^{N_\pm} \,, \tag{4-108}$$

where $N_+(N_-)$ is the number of the basis vectors with $\lambda_2 = 1(-1)$. Consequently, the calculation of the CG coefficients is reduced to a diagonalization of the $n-2$ operators in the eigenspaces $\lambda_2 = \pm 1$ of $C(2)$ separately. This greatly simplifies both the calculation and the tabulation of the CG coefficients. Each CG coefficient table can be decomposed into two sub-tables, one corresponding to $\lambda_2 = 1$ and the other to $\lambda_2 = -1$. See Sec. 4.13 for the tables of CG coefficients.

Example 1: The CG coefficients of S_3. S_3 has three irreps [3], [21] and $[1^3]$. According to (4-90), we only need to calculate the CG coefficients for [21]×[21]. The standard basis of S_3 is

$$\varphi_1^{[21]} = \left| \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 \\ \cline{1-1} \end{array} \right\rangle , \quad \lambda_2^{(1)} = 1 ; \quad \varphi_2^{[21]} = \left| \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 \\ \cline{1-1} \end{array} \right\rangle , \quad \lambda_2^{(1)} = -1 .$$

$$|m_1 m_2\rangle = \varphi_{m_1}^{[21]} \psi_{m_2}^{[21]} .$$

The ordering of the product basis vectors $|m_1 m_2\rangle = \varphi_{m_1}^{[21]} \psi_{m_2}^{[21]}$ is taken as $|11\rangle, |22\rangle, |12\rangle, |21\rangle$. The first two belong to $\lambda_2 = 1$, and the other two belong to $\lambda_2 = -1$. From (4-94) and Table 4.4-2, we obtain the matrix

$$\mathbf{C}(3) = \frac{3}{2} \times \left(\begin{array}{cc|cc} 1 & 1 & & \\ 1 & 1 & & \\ \hline & & -1 & 1 \\ & & 1 & -1 \end{array} \right) . \tag{4-109}$$

The eigenvalues of $\mathbf{C}(3)$ are $\lambda_3 = 3, 0, 0, -3$. Checking those eigenvalues in Fig. 4.5-3, we obtain the CG series

$$[21] \times [21] = [3] + [21] + [1^3] . \tag{4-110}$$

From the eigenequation of $C(3)$, we obtain the CG coefficients, and therefore the coupled basis

$$\Psi_1^{(3)} = \tfrac{1}{\sqrt{2}}(|11\rangle + |22\rangle) , \quad \Psi_{-1}^{(-3)} = \tfrac{1}{\sqrt{2}}(|12\rangle - |21\rangle) .$$
$$\Psi_1^{(0)} = \tfrac{1}{\sqrt{2}}(|11\rangle - |22\rangle) , \quad \Psi_{-1}^{(0)} = -\tfrac{1}{\sqrt{2}}(|12\rangle + |21\rangle) ,$$

It is seen that the irreps (3) and (0), or [3] and [21], belong to the symmetric square, and the irrep (-3), or $[1^3]$, belongs to the anti-symmetric square. In Table 4.13, we use $[\,]_s$ and $[\,]_a$ to represent the symmetric and anti-symmetric squares. Thus Eq. (4-110) is written as

$$[21] \times [21] = [3]_s + [21]_s + [1^3]_a .$$

Example 2: Find the CG coefficients of S_4 for [31] × [22]. The ordering of the product basis vectors $|m_1 m_2\rangle = \varphi_{m_1}^{[31]} \psi_{m_2}^{[22]}$ is taken as

$$|m_1 m_2\rangle = |11\rangle, |21\rangle, |32\rangle; |12\rangle, |22\rangle, |31\rangle .$$

The ordering of the standard basis of S_4 is given in Table 4.4-1. In the above equation, the first three states belong to $\lambda_2 = 1$ and the rest belong to $\lambda_2 = -1$.

Utilizing the matrix elements of [31] and [22] given in Table 4.4-2, it is easy to construct the matrices of $C(3)$ and $C(4)$, namely

$$\begin{array}{cc} \mathbf{C}(4) & \mathbf{C}(3) \end{array}$$

$$\sqrt{2} \left(\begin{array}{ccc|ccc} 0 & 1 & -1 & & & \\ 1 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & & & \\ -1 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & & & \\ \hline & & & 0 & -1 & -1 \\ & & & -1 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ & & & -1 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{array} \right) , \quad \frac{3}{2} \left(\begin{array}{ccc|ccc} 0 & 0 & 0 & & & \\ 0 & 1 & 1 & & & \\ 0 & 1 & 1 & & & \\ \hline & & & 0 & 0 & 0 \\ & & & 0 & -1 & 1 \\ & & & 0 & 1 & -1 \end{array} \right) . \tag{4-111}$$

From the expectation equation of $\mathbf{C}(4)$ one obtains

$$\det|\mathbf{C}(4) - \lambda_4 I| = (\lambda_4 - 2)^3 (\lambda_4 + 2)^3 = 0 .$$

Comparing this with Table 3.2-1, we have

$$[31] \times [22] = [31] + [211] .$$

By diagonalizing $\mathbf{C}(4)$ and $\mathbf{C}(3)$, we obtain the CG coefficients listed in Table 4.13-2b.

Computer calculations of the CG coefficients

The most prominent feature of the EFM for the CG coefficients is that it is easily programmable. The main steps are as follows:

1. For a given $[\nu_1]$ and $[\nu_2]$ note down, from the known CG series $(\nu_1\nu_2\nu)$ [for example from Table 4.10-1 or from the tables given by Itzykson (1966)] and from Table 4.4-1, the eigenvalues $\lambda = k_n\lambda_n + \ldots + k_3\lambda_3$ for the first components of each possible irrep $[\nu]$.

2. Divide the product basis vectors into two groups and calculate the matrices $\mathbf{C}^{(+)}(f)$ in (4-108). We only need to solve the eigenequation of the operator $M = \sum_f k_f C(f)$ in the $\lambda_2 = +1$ subspace, since the first component of all irreps, except the totally anti-symmetric irrep $[1^n]$, correspond to $\lambda_2 = 1$, and the CG coefficients for $[1^n]$ is trivial (see (4-124)).

3. Form the matrices

$$\mathbf{M}^{(+)} = k_n\mathbf{C}^{(+)}(n) + \ldots + k_2\mathbf{C}^{(+)}(3) . \tag{4-112a}$$

Substitute the values λ found in step 1 into the following equation

$$(\mathbf{M}^{(+)} - \lambda\mathbf{I})\mathbf{U}^\tau = 0 , \quad \tau = 1, 2, \ldots, (\nu_1\nu_2\nu) , \tag{4-112b}$$

where $\mathbf{U}^\tau = \{C^{[\nu]\tau,m=1}_{\nu_1 m_1,\nu_2 m_2}\}$ is a column vector with m_1, m_2 as the row index. Solving (4-112b), we find the CG coefficients of first component of the τ-th irrep (ν).

4. The overall phase convention. The phase of the eigenvector $\mathbf{U}^\tau$ is dictated by the overall phase convention, which is stipulated as following: First arrange the product basis vectors $|m_1 m_2\rangle$ according to the order $|1,1\rangle, |1,2,\rangle, \ldots, |1,h_{\nu_2}\rangle, |2,1\rangle, \ldots, |2,h_{\nu_2}\rangle, \ldots |h_{\nu_1}, h_{\nu_2}\rangle$. Then demand that the first non-vanishing component of the vector $\mathbf{U}^\tau$ be positive, that is

$$C^{[\nu]\tau,1}_{\nu_1 m_1,\nu_2 m_2}|_{(m_1,m_2)_{\min}} > 0 , \tag{4-113}$$

where $(m_1 m_2)_{\min}$ means taking the index m_1 as small as possible followed by taking m_2 as small as possible for which the CG coefficient $C^{[\nu]\tau,1}_{\nu_1 m_1,\nu_2 m_2}$ is nonzero.

5. Substituting $\Psi^{[\nu]\tau}_m = \sum_{cd} C^{[\nu]\tau m}_{\nu_1 c,\nu_2 d}|cd\rangle$ into (4-35) and multiplying by $\langle ab|$ from the left, we get

$$C^{[\nu]\tau.m'}_{\nu_1 a,\nu_2 b} = \frac{1}{D^{(\nu)}_{m'm}(T)} \sum_{cd} [D^{(\nu_1)}_{ac}(T) D^{(\nu_2)}_{bd}(T) - D^{(\nu)}_{mm}(T)\delta_{ac}\delta_{bd}] C^{[\nu]\tau,m}_{\nu_1 c,\nu_2 d} . \tag{4-114}$$

Starting from the CG coefficients $C^{[\nu]\tau,1}_{\nu_1 m_1,\nu_2 m_2}$ found using (4-112b), (4-114) and the appropriate transpositions, we can find all other components of the CG coefficients of the τ-th irrep (ν).

Notice that we cannot use the intrinsic quantum number as the multiplicity label for the CG coefficients or for the induction coefficients to be discussed in Sec. 4.15, since in the space of the product states we cannot define a meaningful intrinsic state.

Two EFM programs are available for computing the CG coefficients of the permutation group; one uses the non-recursive method just discussed and the other employs the recursive method (Gao & Chen 1985) to be discussed in Sec. 4.19.

4.12. Properties of the CG Coefficients of Permutation Groups

The CG coefficients of the permutation group have some special properties (Gao & Chen 1985) besides the general results given in Sec. 3.15. These properties can be exploited to reduce the number of independent CG coefficients that have to be calculated, as well as to check the correctness of the calculated CG coefficients.

1. Unitarity

$$\begin{aligned}\sum_{m_1 m_2} C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2} C^{[\nu']\tau',m'}_{\nu_1 m_1,\nu_2 m_2} &= \delta_{\nu\nu'}\delta_{\tau\tau'}\delta_{mm'},\\ \sum_{\nu\tau m} C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2} C^{[\nu]\tau,m}_{\nu_1 m_1',\nu_2 m_2'} &= \delta_{m_1 m_1'}\delta_{m_2 m_2'}.\end{aligned} \tag{4-115}$$

2.

$$C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2} = \varepsilon_1(\nu_1\nu_2\nu_\tau) C^{[\nu]\tau,m}_{\nu_2 m_2,\nu_1 m_1} \ . \tag{4-116a}$$

From the overall phase convention (4-113), it is seen that

$$\varepsilon_1(\nu_1\nu_2\nu_\tau) = \mathrm{sign}(C^{[\nu]\tau,1}_{\nu_1 m_1,\nu_2 m_2}|_{(m_2 m_1)_{\min}}) \ , \tag{4-116b}$$

where $(m_2 m_1)_{\min}$ means that we first take the index m_2 as small as possible and then take m_1 as small as possible.

For $\nu_1 = \nu_2$ let

$$\delta_{\nu_\tau} = \varepsilon_1(\nu_1\nu_1\nu_\tau) \ . \tag{4-116c}$$

If $\delta_{\nu_\tau} = 1\ (-1)$, then the irrep $[\nu]_\tau$ belongs to the symmetric (anti-symmetric) square $[(\nu_1)\times(\nu_2)]_s([(\nu_1)\times(\nu_2)]_a)$.

3. From (3-327b) we have, for $\nu_1 \neq \nu_2 \neq \nu \neq \nu_1$,

$$\frac{1}{\sqrt{h_\nu}} C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2,m_2} = \varepsilon_2(\nu_1\nu_2\nu_\tau)\frac{1}{\sqrt{h_{\nu_1}}} C^{[\nu_1]\tau,m_1}_{\nu m,\nu_2 m_2} = \varepsilon_3(\nu_1\nu_2\nu_\tau)\frac{1}{\sqrt{h_{\nu_2}}} C^{[\nu_2]\tau,m_2}_{\nu_1 m_1,\nu m} \ , \tag{4-117}$$

with the phase factor

$$\varepsilon_2(\nu_1\nu_2\nu_\tau) = \mathrm{sign}(C^{[\nu]\tau,m}_{\nu_1 1,\nu_2 m_2}|_{(m m_2)=\min}) \ , \tag{4-118}$$

$$\varepsilon_3(\nu_1\nu_2\nu_\tau) = \mathrm{sign}(C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 1}|_{(m_1 m)=\min}) \ . \tag{4-119}$$

4. For $\nu_1 = \nu_2 \neq \nu$, (4-117) still holds. We also have

$$C^{[\nu_1]\tau,m_1}_{\nu m,\nu_1 m_2} = \delta_{\nu_\tau} C^{[\nu_1]\tau,m_2}_{\nu m,\nu_1 m_1} \ , \quad \delta_{\nu_\tau} = \varepsilon_1(\nu_1\nu_1\nu_\tau) \ , \tag{4-120}$$

which can be proved using (4-116c) and (4-117).

5. The symmetries for $\nu_1 = \nu_2 = \nu$ are more involved (see Gao & Chen 1985).

6. The symmetries of the CG coefficients under conjugation are

$$\begin{aligned}C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2} &= \varepsilon_4(\nu_1\nu_2\nu_\tau)\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2} C^{[\nu]\tau,m}_{\tilde\nu_1 \tilde m_1,\tilde\nu_2 \tilde m_2}\\ &= \varepsilon_5(\nu_1\nu_2\nu_\tau)\Lambda^{\nu_1}_{m_1}\Lambda^{\nu}_{m} C^{[\tilde\nu]\tau,\tilde m}_{\tilde\nu_1 \tilde m_1,\nu_2 m_2} = \varepsilon_6(\nu_1\nu_2\nu_\tau)\Lambda^{\nu_2}_{m_2}\Lambda^{\nu}_{m} C^{[\tilde\nu]\tau,\tilde m}_{\nu_1 m_1,\tilde\nu_2 \tilde m_2} \ ,\end{aligned} \tag{4-121}$$

$$\varepsilon_4(\nu_1\nu_2\nu_\tau) = \mathrm{sign}(\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2} C^{[\nu]\tau,1}_{\nu_1 m_1,\nu_2 m_2}|_{(\overline{m}_1\overline{m}_2)}) \ , \tag{4-122a}$$

$$\varepsilon_5(\nu_1\nu_2\nu_\tau) = \mathrm{sign}(\Lambda^{\nu_1}_{m_1}\Lambda^{\nu}_{m} C^{[\nu]\tau,h_\nu}_{\nu_1 m_1,\nu_2 m_2}|_{(\overline{m}_1\underline{m}_2)}) \ , \tag{4-122b}$$

$$\varepsilon_6(\nu_1\nu_2\nu_\tau) = \mathrm{sign}(\Lambda^{\nu_2}_{m_2}\Lambda^{\nu}_{m} C^{[\nu]\tau,h_\nu}_{\nu_1 m_1,\nu_2 m_2}|_{(\underline{m}_1,\overline{m}_2)}) \ , \tag{4-122c}$$

where $(\overline{m}_1\overline{m}_2)$ means first taking the index m_1 as large as possible and then taking m_2 as large as possible, whereas $(\overline{m}_1\underline{m}_2)$ means taking m_1 as large as possible and then taking m_2 as small as possible.

Notice that for non-multiplicity free cases, (4-121) in general only holds when the partitions $[\nu_1]$ and $[\nu_2]$ (or $[\nu_1]$ and $[\nu]$, or $[\nu_2]$ and $[\nu]$) are not simultaneously self-conjugate. If both are self-conjugate (for S_n with $n \leq 7$, then they must equal), the imposition of the symmetry

$$C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_1 m_2} = \pm\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_1}_{m_2} C^{[\nu]\tau,m}_{\nu_1 \tilde{m}_1,\nu_1 \tilde{m}_2}, \quad \text{for} \quad [\nu_1] = [\tilde{\nu}_1] \neq [\nu] \,, \tag{4-123a}$$

or

$$C^{[\nu]\tau,m}_{\nu_1 m_1,\nu m_2} = \pm\Lambda^{\nu}_{m_2}\Lambda^{\nu}_{m} C^{[\nu]\tau,\tilde{m}}_{\nu_1 m_1,\nu \tilde{m}_2} \quad \text{for} \quad [\nu] = [\tilde{\nu}] \neq [\nu_1] \,, \tag{4-123b}$$

will be of help for the multiplicity separation.

For multiplicity-free cases, the symmetries (4-116)–(4-123) are satisfied automatically, however the phases now enter of necessity instead of being determined by the phase convention. For non-multiplicity-free cases, the symmetries (4-116a), (4-120) and (4-123) are imposed to reduce the arbitrariness in the multiplicity separation and to yield simpler numerical values for the CG coefficients.

If among $[\nu_1], [\nu_2]$ and $[\nu]$, one is totally symmetric, $[n]$, or totally anti-symmetric, $[1^n]$, then the CG coefficients are very simple. From (4-90) and (4-121) we have

$$\begin{aligned}
C^{[\nu]m}_{[\nu_1]m_1,[n]1} &= \delta_{\nu\nu_1}\delta_{mm_1} \,. \\
C^{[n],1}_{[\nu_1]m_1,[\nu_2]m_2} &= \frac{1}{\sqrt{h_{\nu_1}}}\delta_{\nu_1\nu_2}\delta_{m_1 m_2} \,. \\
C^{[\tilde{\nu}]\tilde{m}}_{[\nu_1]m_1,[1^n]1} &= \Lambda^{\nu_1}_{m_1}\delta_{\nu_1\nu}\delta_{m_1 m} \,. \\
C^{[1^n]1}_{[\nu_1]m_1,[\tilde{\nu}]_2\tilde{m}_2} &= \frac{1}{\sqrt{h_{\nu_1}}}\Lambda^{\nu_1}_{m_1}\delta_{\nu_1\nu_2}\delta_{m_1 m_2} \,.
\end{aligned} \tag{4-124}$$

From this the totally symmetric or anti-symmetric state is expressed as

$$\begin{aligned}
\Psi^{[n]} &= \frac{1}{\sqrt{h_\nu}}\sum_m \varphi^{[\nu]}_m(x)\psi^{[\nu]}_m(\xi) \,, \\
\Psi^{[1^n]} &= \frac{1}{\sqrt{h_\nu}}\sum_m \Lambda^{\nu}_m\varphi^{[\nu]}_m(x)\psi^{[\tilde{\nu}]}_{\tilde{m}}(\xi) \,.
\end{aligned} \tag{4-125}$$

The symmetry relation given above can be checked using the CG coefficients given in Sec. 4.13. For example, (4-117) can be checked using Table 4.13-3e and 4.13-3f:

$$\frac{1}{\sqrt{6}}C^{[311]\tau,2}_{[311]1,[32]2} = \frac{1}{\sqrt{5}}C^{[32]\tau,2}_{[311]1,[311]2} \,, \quad \frac{1}{\sqrt{6}}\begin{pmatrix} -\frac{1}{\sqrt{10}} \\ -\frac{1}{\sqrt{60}} \end{pmatrix} = \frac{1}{\sqrt{5}}\begin{pmatrix} -\frac{1}{\sqrt{12}} \\ -\frac{1}{\sqrt{72}} \end{pmatrix} \,, \quad \tau = \begin{cases} \alpha \\ \beta \end{cases} .$$

Similarly, (4-123) can be checked by the following example:

$$C^{[221]\tau,5}_{[311]1,[311]6} = C^{[\bar{3}2]\tau,\bar{1}}_{[311]1,[311]\bar{1}} = \varepsilon_6\Lambda^{[32]}_1\Lambda^{[311]}_1 C^{[32]\tau,1}_{[311]1,[311]1} = \begin{pmatrix} \sqrt{\frac{4}{12}} \\ -\sqrt{\frac{4}{72}} \end{pmatrix} \,, \quad \tau = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} .$$

4.13. Tables of the CG Coefficients for S_3-S_5

Two sets of CG coefficients for the permutation group S_2–S_6 have been produced. One was computed by Schindler (1978), where only the CG coefficients for the so-called working triplets of irreps are calculated. The other was computed by Chen & Gao (1981). All the CG coefficients of S_2–S_6, except those for $[321] \times [321] \to [321]^5$ have been published, along with the program used to calculate them.

The absolute phase of the permutation group CG coefficients tabulated in Schindler (1968) and Chen & Gao (1981) are all chosen randomly.

We have now adopted the phase convention (4-113) for reasons to be explained in Sec. 7.16. The CG coefficients of S_3–S_5 are listed in Tables 4.13-1 to 4.13-3. The CG coefficients for $[321] \times [321] \to [321]^5$ are given in Gao & Chen (1985), the CG coefficients for the remaining Kronecker product of S_6 can be calculated from the $S_6 \supset S_5$ isoscalar factors (Chen, Gao, Shi 1984) and the S_5 CG coefficient Table given in this section.

The CG coefficients tabulated here and in Gao & Chen (1985) differ from the Schindler (1968) results in the following respects. (a) Ours have a consistent absolute phase convention. (b) Our multiplicity separation is based, whenever possible, on the imposition of the symmetries, while theirs is based on an *ad hoc* choice. (c) Our tables give the exact values of the coefficients instead of the approximate values to 16 decimal places.

Some remarks on Table 4.13 are now in order:

1. Each table with a given $[\nu_1]$ and $[\nu_2]$ is divided into two tables according to the values of λ_2, with that $\lambda_2 = 1(-1)$ part at the upper (lower) half of the table.

2. The second column N gives the normalization factors. The values listed in the tables are the squares of the CG coefficients. The asterisk denotes a negative CG coefficient and a blank denotes a zero CG coefficient. For example, from Table 4.13-3b we have

$$C^{[41]2}_{[41]3,[32]2} = \left\langle \begin{array}{|c|c|c|c|}\hline 1&2&3&5\\\hline 4\\\cline{1-1}\end{array} \;\middle|\; \begin{array}{|c|c|c|c|}\hline 1&2&4&5\\\hline 3\\\cline{1-1}\end{array} \;\; \begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3&5\\\cline{1-2}\end{array} \right\rangle = -\frac{1}{\sqrt{45}} .$$

3. Each table can be read either horizontally or vertically, for example, from Table 4.13-3b one has

$$\Psi^{[41]}_2 = \frac{1}{\sqrt{45}}\Big(\sqrt{15}\varphi^{[41]}_1\psi^{[32]}_1 + \sqrt{4}\varphi^{[41]}_2\psi^{[32]}_1 - \varphi^{[41]}_3\psi^{[32]}_2 + \sqrt{12}\varphi^{[41]}_3\psi^{[32]}_4 - \varphi^{[41]}_4\psi^{[32]}_3 + \sqrt{12}\varphi^{[41]}_4\psi^{[32]}_5\Big) ,$$

$$\varphi^{[41]}_1\psi^{[32]}_4 = -\sqrt{\frac{18}{48}}\Psi^{[32]}_4 + \sqrt{\frac{10}{16}}\Psi^{[221]}_1 .$$

4. In the sub-tables 3e and 3f, α and β are the multiplicity labels, for example, $[311\alpha]$ and $[311\beta]$ represent $[311]$ $\tau = \alpha$ and $[311]\tau = \beta$, respectively.

5. Using the symmetries given in Sec. 4.12, we can obtain the other CG coefficients not listed in the tables. The phase factors Λ^{ν}_{m} are given in Table 4.4-1.

Table 4.13. Tables of the CG coefficients of the permutation groups $S_3 - S_6$.*

S_3 1 $[21] \times [21] = [3]_s + [21]_s + [1^3]_a$

	N	(11)	(22)
[3]	2	1	1
[21]1	2	1	*1
		(12)	(21)
[21]2	2	*1	*1
$[1^3]$	2	1	*1

S_4 2a $[31] \times [31] = [4]_s + [31]_s + [22]_s + [211]_a$

	N	(11)	(12)	(21)	(22)	(33)
[4]	3	1			1	1
[31]1	6	4			*1	*1
2	6		*1	*1	2	*2
[22]1	2		2	2	1	*1
[211]1	2		1	*1		
		(13)	(31)	(23)	(32)	
[31]3	6	*1	*2	*2	*2	
[22]2	6	2	2	*1	*1	
[211]2	2	1	*1			
3	2			1	*1	

*$[\nu]_s$ denotes the representation belongs to the symmetric product $[[\nu_1] \times [\nu_1]]_s$, $[\nu]_a$ denotes the representation belongs to the antisymmetric product $[[\nu_1] \times [\nu_1]]_a$.

cont'd

S_4 2b $[31] \times [22] = [31] + [211]$

	N	(11)	(21)	(32)
[31]1	2		1	1
2	4	2	1	*1
[211]1	4	2	*1	1
		(12)	(22)	(31)
[31]3	4	2	*1	*1
[211]2	4	2	1	1
3		*1	1	

S_4 2c $[22] \times [22] = [4]_s + [22]_s + [1^4]_a$

	N	(11)	(22)
[4]	2	1	1
[22]1	2	1	*1
		(12)	(21)
[22]2	2	*1	*1
$[1^4]$	2	1	*1

S_5 3a $[41] \times [41] = [5]_s + [41]_s + [32]_s + [311]_a$

	N	(11)	(12)	(13)	(21)	(22)	(23)	(31)	(32)	(33)	(44)
[5]	4	1				1				1	1
[41]1	12	9				*1				*1	*1
2	36		*3		*3	20				*5	*5
3	36			*3			*5	*3	*5	10	*10
[32]1	36		15		15	4				*1	*1
2	36			15			*1	15	*1	2	*2
4	6						2		2	1	*1
[311]1	2		1		*1						
2	2			1				*1			
4	2						1		*1		
		(14)	(24)	(34)	(41)	(42)	(43)				
[41]4	36	*3	*5	*10	*3	*5	*10				
[32]3	36	15	*1	*2	15	*1	*2				
5	6			2	*1		2	*1			
[311]3	2	1			*1						
5	2		1			*1					
6	2			1			*1				

S_5 3b $[41] \times [32] = [41] + [32] + [311] + [221]$

	N	(11)	(12)	(14)	(21)	(22)	(24)	(31)	(32)	(34)	(43)	(45)
[41]1	3				1				1		1	
2	45	15			4				*1	12	*1	12
3	45		15			*1	12	*1	2	6	*2	*6
[32]1	72	12			20				*5	*15	*5	*15
2	144		24			*10	*30	*10	20	*15	*20	15
4	48			*18		*10		*10	*5		5	
[311]1	40	20			*12				3	*1	3	*1
2	80		40			6	*2	6	*12	*1	12	1
4	16					*2	6	2		*3		3
[221]1	16			10		*2		*2	*1		1	
3	16					6	2	*6		*1		1
		(13)	(15)	(23)	(25)	(33)	(35)	(41)	(42)	(44)		
[41]4	45	15		*1	12	*2	*6	*1	*2	*6		
[32]3	144	24		*10	*30	*20	15	*10	*20	15		
5	48		*18	*10		5		*10	5			
[311]3	80	40		6	*2	12	1	6	12	1		
5	16			*2	6		3	2		3		
6	8					*1	*3		1	3		
[221]2	16		10	*2		1		*2	1			
4	16			6	2		1	*6		1		
5	8					3	*1		*3	1		

cont'd

S_5 3c $[311]\times[41]=[41]+[32]+[311]+[221]+[21^3]$

	N	(11)	(12)	(13)	(21)	(22)	(23)	(34)	(41)	(42)	(43)	(54)	(64)
[41]1	3		1				1	1					
2	3	*1									1	1	
3	3				*1					*1			1
[32]1	48	20	*12				3	3			5	5	
2	48			3	20	3	*6	6		*5			5
4	96			*2		*2	*1	1		30	*15	15	30
[311]1	48	12	20				*5	*5			3	3	
2	48			*5	12	*5	10	*10		*3			3
4	48			3		*3			*12	5	10	*10	5
[221]1	96			30		30	15	*15		2	*1	1	2
3	48			*5		5			20	3	6	*6	3
$[21^3]1$	3			1		*1			1				
		(14)	(24)	(31)	(32)	(33)	(44)	(51)	(52)	(53)	(61)	(62)	(63)
[41]4	3			*1					*1				*1
[32]3	48	3	6	20	3	6			*5				*5
5	96	*2	1		*2	1	15		30	15			*30
[311]3	48	*5	*10	12	*5	*10			*3				*3
5	48	3			*3		*10	*12	5	*10			*5
6	48		3			*3	5			*5	*12	*20	
[221]2	96	30	*15		30	*15	1		2	1			*2
4	48	*5			5		*6	20	3	*6			*3
5	48		*5			5	3			*3	20	*12	
$[21^3]2$	3	1			*1			1					
3	3		1			*1					1		
4	3						1			*1		1	

S_5 3d $[32]\times[32]=[5]_s+[41]_s+[32]_s+[311]_a+[221]_s+[21^3]_a$

	N	(11)	(12)	(14)	(21)	(22)	(24)	(33)	(35)	(41)	(42)	(44)	(53)	(55)
[5]	5	1				1		1				1		1
[41]1	30	4				4		4				*9		*9
2	18	4				*1	*3	*1	*3		*3		*3	
3	36		*2	*6	*2	4	*3	*4	3	*6	*3		3	
[32]1	36	16				*4	3	*4	3		3		3	
2	72		*8	6	*8	16	3	*16	*3	6	3		*3	
4	24		2		2	1		*1				9		*9
[311]1	4						1		1		*1		*1	
2	8			2			1		*1	*2	*1		1	
4	40		8	6	*8		*3		3	*6	3		*3	
[221]1	8		2		2	1		*1				*1		1
3	8			2			*1		1	2	*1		1	
$[21^3]1$	20		6	*2	*6		1		*1	2	*1		1	
		(13)	(15)	(23)	(25)	(31)	(32)	(34)	(43)	(45)	(51)	(52)	(54)	
[41]4	36	*2	*6	*4	3	*2	*4	3	3		*6	3		
[32]3	72	*8	6	*16	*3	*8	*16	*3	*3		6	*3		
5	24	2		*1		2	*1			*9			*9	
[311]3	8		2		*1			*1	1		*2	1		
5	40	8	6		3	*8		3	*3		*6	*3		
6	20			4	*3		*4	3	*3			3		
[211]2	8	2		*1		2	*1			1			1	
4	8		2		1			1	1		2	1		
5	4				*1			1	1			*1		
$[21^3]2$	20	6	*2		*1	*6		*1	1		2	1		
3	10			3	1		*3	*1	1			*1		
4	2									1			*1	

cont'd

S_5 3e $[311]\times[32]=[41]+[32]+[311]^2+[221]+[21^3]$

	N	(11)	(12)	(14)	(21)	(22)	(24)	(33)	(35)	(41)	(42)	(44)	(53)	(55)	(63)	(65)
[41]1	3	1				1		1								
2	60	*12				3	*1	3	*1		*5	15	*5	15		
3	120		6	*2	6	*12	*1	12	1	10		*15		15	*10	*30
[32]1	24						5		5		4	3	4	3		
2	48			10			5		*5	*8		*3		3	8	*6
4	48		*10		*10	*5		5		*6	3		*3		*6	
[311α]1	40	16				*4	*3	*4	*3			5		5		
2	80		*8	*6	*8	16	*3	*16	3			*5		5		*10
4	80			10			*5		5	*8	*16	3	16	*3	*8	*6
[311β]1	60	4				*1	12	*1	12		*15		*15			
2	60		*1	12	*1	2	6	*2	*6	15					*15	
4	60		*15		15					1	2	6	*2	*6	1	*12
[221]1	48		6		6	3		*3		*10	5		*5		*10	
3	48		8	*6	*8		3		*3			5		*5		*10
[21^3]1	120		10	30	*10		*15		15	6	12	1	*12	*1	6	*2
		(13)	(15)	(23)	(25)	(31)	(32)	(34)	(43)	(45)	(51)	(52)	(54)	(61)	(62)	(64)
[41]4	120	6	*2	12	1	6	12	1		15	10		15		10	30
[32]3	48		10		*5			*5		3	*8		3		*8	6
5	48	*10		5		*10	5		*3		*6	*3			6	
[311α]3	80	*8	*6	*16	3	*8	*16	3		5			5			10
5	80		10		5			5	16	*3	*8	16	*3		8	6
6	40				*5			5	*4	*3		4	3	16		
[311β]3	60	*1	12	*2	*6	*1	*2	*6			15				15	
5	60	*15				15			*2	*6	1	*2	*6		*1	12
6	60			*15			15		1	*12		*1	12	*4		
[221]2	48	6		*3		6	*3		*5		*10	*5			10	
4	48	8	*6		*3	*8		*3		*5			*5			10
5	24			4	3		*4	*3		*5			5			
[21^3]2	120	10	30		15	*10		15	*12	*1	6	*12	*1		*6	2
3	60			5	*15		*5	15	3	*1		*3	1	*12		
4	3								*1			1		*1		

cont'd

S_6 $3f$ $[311]\times[311]=[5]_s+[41]_s+[32]^2_s+[311]_a+[221\alpha]_s+[221\beta]_a+[21^3]_a+[1^5]_s$

	N	(11)	(12)	(14)	(21)	(22)	(24)	(33)	(35)	(36)	(41)	(42)	(44)	(53)	(55)	(56)	(63)	(65)	(66)
[5]	6	1				1		1					1		1				1
[41]1	6	1				1		1					*1		*1				*1
2	72	20				*5	*3	*5	*3			*3	5	*3	5				*20
3	72		*5	3	*5	10		*10		*3	3		10		*10	*5	*3	*5	
[32α]1	12	4				*1		*1					*1		*1				4
2	12		*1		*1	2		*2					*2		2	1		1	
4	96		*6	10	*6	*3	*5	3	5	10	10	*5	3	5	*3	6	10	6	
[32β]1	72	4				*1	15	*1	15			15	1	15	1				*4
2	72		*1	*15	*1	2		*2		15	*15		2		*2	*1	15	*1	
4	12		2		2	1		*1					1		*1	2		2	
[311]1	4						1		1			*1		*1					
2	4			*1						1	1						*1		
4	4		1		*1											1		*1	
[221α]1	96		10	6	10	5	*3	*5	3	6	6	*3	*5	3	5	*10	6	*10	
3	12			*1			*2		2	*1	*1	*2		2			*1		
[221β]1	12			2			*1		1	2	*2	1		*1			*2		
3	72		*15	1	15		2		*2	1	*1	*2		2		15	*1	*15	
[21^3]1	72		3	5	*3		10		*10	5	*5	*10		10		*3	*5	3	
		(13)	(15)	(16)	(23)	(25)	(26)	(31)	(32)	(34)	(43)	(45)	(46)	(51)	(52)	(54)	(61)	(62)	(64)
[41]4	72	*5	3		*10		3	*5	*10			*10	5	3		*10		3	5
[32α]3	12	*1			*2			*1	*2			2	*1			2			*1
5	96	*6	10		3	5	*10	*6	3	5	5	*3	*6	10	5	*3		*10	*6
[32β]3	72	*1	*15		*2		*15	*1	*2			*2	1	*15		*2		*15	1
5	12	2			*1			2	*1			*1	*2			*1			*2
[311]3	4		*1				*1							1				1	
5	4	1						*1					*1						1
6	4				1				*1			1				*1			
[221α]2	96	10	6		*5	3	*6	10	*5	3	3	5	10	6	3	5		*6	10
4	12		*1			2	1			2	2			*1	2			1	
5	12			4		1				*1	*1				1		4		
[221β]2	12		2			1	*2			1	*1			*2	*1			2	
4	72	*15	1			*2	*1	15		*2	2		*15	*1	2			1	15
5	72			*4	*15	*1			15	1	*1	15			1	*15	4		
[21^2]2	72	3	5			*10	*5	*3		*10	10		3	*5	10			5	*3
3	72			*20	3	*5			*3	5	*5	*3			5	3	20		
4	6			1		*1				1	*1				1		*1		
[1^5]	6			1		*1				1	1				*1		1		

4.14. Outer–Product of the Permutation Group and the Littlewood Rule

Suppose that there are two subsystems with identical particles $1,2,\ldots,n_1$ and $n_1+1,\ldots n_1+n_2=n$ which have the permutation symmetry $[\nu_1]$ and $[\nu_2]$, respectively. The question posed in this section is how to construct a wave function of the total system with the permutation symmetry $[\nu]$. Let the wave functions of these two subsystems be denoted as follows:

$$\begin{aligned}
&\psi^{[\nu_1]}_{m_1}(1,2,\ldots,n_1)=\psi^{[\nu_1]}_{m_1}(\omega^0_1)=|Y^{[\nu_1]}(\omega^0_1)\rangle\ ,\\
&\psi^{[\nu_2]}_{m_2}(n_1+1,\ldots,n)=\psi^{[\nu_2]}_{m_2}(\omega^0_2)=|Y^{[\nu_2]}_{m_2}(\omega^0_2)\rangle\ .\\
&(\omega^0_1)=(1,2,\ldots,n_1),\quad (\omega^0_2)=(n_1+1,\ldots,n)\ ,\\
&m_1=1,2,\ldots,h_{\nu_1},\quad m_2=1,2,\ldots,h_{\nu_2}\ .
\end{aligned}\tag{4-126}$$

They are the Yamanouchi basis of the permutation groups $S_{n_1}=S_{n_1}(1,2,\ldots,n_1)$ and $S_{n_2}=S_{n_2}(n_1+1,\ldots,n)$, respectively. $Y^{(\nu_i)}_{m_i}(\omega^0_i)$ represents a Young tableau associated with the number (ω^0_i): Their products are denoted by

$$\begin{aligned}
&|m_1m_2\omega^0\rangle=\psi^{[\nu_1]}_{m_1}(\omega^0_1)\psi^{[\nu_2]}_{m_2}(\omega^0_2)=|Y^{[\nu_1]}_{m_1}(\omega^0_1)Y^{[\nu_2]}_{m_2}(\omega^0_2)\rangle,\\
&(\omega^0)=(\omega^0_1,\omega^0_2)=(1,2,\ldots n)\ .
\end{aligned}\tag{4-127}$$

For example

$$|Y^{[21]}_1(123)\rangle=\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}\right\rangle\quad |Y^{[21]}_2(456)\rangle=\left|\begin{array}{|c|c|}\hline 4&6\\\hline 5\\\cline{1-1}\end{array}\right\rangle\ .\tag{4-128}$$

Define $h_3=\binom{n}{n_1}$ *normal order sequences*,

$$\begin{aligned}
&(\omega)=(\omega_1,\omega_2)\quad (\omega_1)=(a_1a_2\ldots a_{n_1}),\quad (\omega_2)=(a_{n_1+1}\ldots a_n)\ ,\\
&a_1<a_2<\ldots<a_{n_1},\ a_{n_1+1}<a_{n_1+2}<\ldots<a_n\ .
\end{aligned}\tag{4-129}$$

The a_i each represents any one of the numbers 1,2,...,n. For example $n_1=3,n_2=2,h_3=\binom{5}{3}=10$. The ten normal order sequences are listed in Table 4.14-1.

Table 4.14-1. Normal order sequences (ω) with their ordinals and parity δ_ω.

$\omega(\delta\omega)$	1(+)	2(−)	3(+)	4(−)	5(+)	6(−)	7(+)	8(+)	9(−)	10(+)
(ω)	(123,45)	(124,35)	(134,25)	(234,15)	(125,34)	(135,24)	(235,14)	(145,23)	(245,13)	(345,12)

The ordering of the sequences (ω) is specified in the following way. We regard the part (ω_1) in $(\omega)=(\omega_1,\omega_2)$ as a vector of length n_1. If the last nonzero component of the vector $(\omega_1)-(\overline{\omega}_1)$ is less than zero, then we say that $(\omega)<(\overline{\omega})$. The motivation for this ordering is to ensure that the ordering of the totally symmetric Gel'fand basis vector $\psi^{[n_1]}(\omega_1)$ is consistent with the convention in Sec. 7.4. To each normal order sequence (ω) we associated a parity factor $\delta_\omega,\delta_\omega(=\pm1)$ being the parity of the permutation operator which transforms the normal order sequence (ω^0) into (ω).

The *left coset* decomposition of S_n with respect to the subgroup $S_{n_1}\times S_{n_2}$ is denoted by [cf. (2-106b)],

$$S_n=\sum_{\omega=1}^{h_3}Q_\omega(S_{n_1}\times S_{n_2})\ ,\tag{4-130}$$

where the left coset representatives Q_ω are just the so-called *order-preserving permutation* (MacFarlane 1960),

$$Q_\omega = \begin{pmatrix} \omega^0 \\ \omega \end{pmatrix}, \quad Q_\omega(\omega^0) = (\omega) \ . \tag{4-131}$$

Applying the h_3 Q_ω's to (4-127), we get altogether $N = h_{\nu_1} h_{\nu_2} h_3$ basis vectors

$$\begin{aligned} Q_\omega |m_1 m_2 \omega^0\rangle &= |m_1 m_2 \omega\rangle \\ &= \psi^{[\nu_1]}_{m_1}(\omega_1)\psi^{[\nu_2]}_{m_2}(\omega_2) = |Y^{[\nu_1]}_{m_1}(\omega_1) Y^{[\nu_2]}_{m_2}(\omega_2)\rangle \ , \\ m_i &= 1, 2, \ldots, h_{\nu_i}, \quad \omega = 1, 2, \ldots, h_3 \ , \end{aligned} \tag{4-132}$$

where $Y^{[\nu_i]}_{m_i}(\omega_i)$ denotes a generalized Young tableau formed by filling the Young diagram $[\nu_i]$ with the numbers (ω_i) according to the order specified by the Yamanouchi symbol m_i.

Now let us investigate the condition for these N states to be linearly independent. In Sec. 4.7, it was pointed out that the quantum numbers $(\nu_i m_i)$ are not sufficient to specify the basis functions $\psi^{[\nu_i]}_{m_i}$ uniquely. In addition to $(\nu_i m_i)$, we need the Weyl tableaux W_i. Therefore, to be precise, (4-132) should be rewritten as

$$|m_1 m_2 \omega\rangle = \psi^{[\nu_1]}_{m_1}(\omega_1, W_1)\psi^{[\nu_2]}_{m_2}(\omega_2, W_2). \tag{4-133}$$

The vectors of (4-133) are orthogonal in the quantum numbers m_1 and m_2, but not necessarily in ω, unless all the single particle states in the Weyl tableau W_1 are different from those in W_2. Under the above condition we have

$$\langle m_1' m_2' \omega' | m_1 m_2 \omega\rangle = \delta_{m_1 m_1'} \delta_{m_2 m_2'} \delta_{\omega\omega'} \ , \tag{4-134}$$

that is, the N basis vectors are orthonormal. If there is any overlap between the single particle states in W_1 and those in W_2, the number of independent basis vectors will be less than N (see Sec. 4.17). In the following we assume that (4-134) is true. According to Sec. 2.10, the N basis vectors of (4-132) carry the induced rep of S_n, $([\nu_1] \times [\nu_2]) \uparrow S_n$, which is also called the outer-product of the irreps $[\nu_1]$ and $[\nu_2]$, denoted as $[\nu_1] \otimes [\nu_2]$. It is a reducible rep of S_n. The decomposition of the induced rep into irreps of S_n, [see (2-106f)]

$$([\nu_1] \times [\nu_2]) \uparrow S_n = \sum_\nu \{\nu_1 \nu_2 \nu\} [\nu] \ , \tag{4-135}$$

where the integers $\{\nu_1 \nu_2 \nu\}$ are the number of times $[\nu]$ occurs in the induced rep, is determined by the *Littlewood rule* (or the *outer-product reduction rule*, also known as the *Littlewood–Richardson rule*):

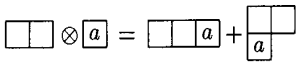
1. Draw the Young diagrams $[\nu_1]$ and $[\nu_2]$.

2. Among these two, choose the more complicated Young diagram as the base (this is just for convenience, in principle we may choose either one as the base), and fill up the other Young diagram with a's in the first row, b's in the second and so on.

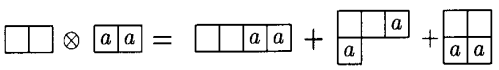
3. Add the boxes labelled a to the base Young diagram, and enlarge the base diagram in all possible ways subject to the rule that no two a's appear in the same column and that the resultant diagram be regular.

4. Repeat the process with the boxes labelled b, under the further restriction that at no stage does the total number of b's exceed the total number of a's counting from right to left and from top to bottom. Then continue the process in the same way with c, d, and so on.

5. The final number of Young diagrams $[\nu]$ formed in this way gives the coefficient $\{\nu_1\nu_2\nu\}$ in the Littlewood rule (4-135).

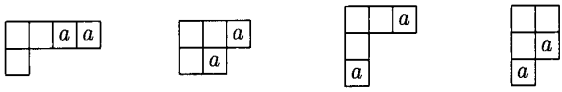
Example 1:  .

Therefore $[2]\otimes[1] = [3] + [21]$.

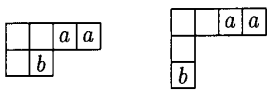
Example 2:  .

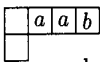
Thus $[2]\otimes[2] = [4] + [31] + [22]$. Notice that $[2] \times [2] \neq ([2] \otimes [1]) \otimes [1]$.

Example 3: Outer-product reduction of $[21]\times[21]$. The base Young diagram is  , and the second Young diagram is  . According to step 3, we have the following enlarged Young diagrams.

(1) 

Adding to the box labelled b to (i) we get the following two diagrams,

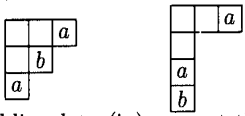
(2) 

Notice that the diagram  is not permissible, since the letter sequence read from this diagram is (baa) so that b occurs before a. On the other hand, from (ii) we have

(3) 

Here the first diagram is permissible, since the letter sequence is (aba).

From (iii), we have

(4) 

Similarly, adding b to (iv), we get the diagrams [222] and [2211]. Finally we have the required result:

$$[21] \otimes [21] = [42] + [411] + [33] + 2[321] + [31^3] + [2^3] + [2^2 1^2] \ . \tag{4-136}$$

Itzykson (1966) has calculated the values $\{\nu_1\nu_2\nu\}$ for S_n with $n \leq 8$. Since the total dimension of both sides of (4-135) must be equal, one has

$$h_{\nu_1} h_{\nu_2} h_3 = \sum_{\nu} \{\nu_1\nu_2\nu\} h_\nu . \tag{4-137}$$

This equation provides a useful check for the calculation of the Littlewood rule.

We will prove later that (4-135) also holds when all the Young diagrams are replaced by their conjugate diagrams:

$$[\tilde{\nu}_1] \otimes [\tilde{\nu}_2] = \sum_{\tilde{\nu}} \{\nu_1\nu_2\nu\} [\tilde{\nu}] . \tag{4-138}$$

Table 4.14-2 gives the outer-product reduction rule for S_3–S_5.

Table 4.14-2. Outer–Product Reduction Rule. The left(right) heading matches the top(bottom) one.

S_3 group

	[3]	[21]	
[2]⊗[1]	1	1	[11]⊗[1]
	[1³]	[21]	

S_4 group

	[4]	[31]	[22]	[211]	[1⁴]	
[3]⊗[1]	1	1				[1³]⊗[1]
[21]⊗[1]		1	1	1		
[2]⊗[2]	1	1	1	1		[1²]⊗[1²]
[2]⊗[11]		1		1		
	[1⁴]	[211]	[22]	[31]	[4]	

S_5 group

	[5]	[41]	[32]	[311]	[221]	[21³]	[1⁵]	
[4]⊗[1]	1	1						[1⁴]⊗[1]
[31]⊗[1]		1	1	1				[211]⊗[1]
[22]⊗[1]			1		1	1		
[3]⊗[2]	1	1	1					[1³]⊗[11]
[21]⊗[2]		1	1	1	1			[21]⊗[11]
[3]⊗[11]		1		1				[1³]⊗[2]
	[1⁵]	[21³]	[2²1]	[311]	[32]	[41]	[5]	

Ex. 4.6. Use the Littlewood rule to check the outer–product reduction for S_5.

4.15. The Calculation of the Induction Coefficients (IDC) of S_n

The N basis vectors of (4-132) can be combined linearly into the irreducible basis of S_n

$$\Psi_m^{[\nu]\tau} = \sum_{m_1 m_2 \omega} C^{[\nu]\tau,m}_{\nu_1 m_1 \omega_1, \nu_2 m_2 \omega_2} |m_1 m_2 \omega\rangle \ , \tag{4-139}$$

where the coefficients

$$C^{[\nu]\tau,m}_{\nu_1 m_1 \omega_1, \nu_2 m_2 \omega_2} \equiv C^{[\nu]\tau,m}_{\nu_1 m_1, \nu_2 m_2, \omega} \ , \tag{4-140}$$

are called the $([\nu_1]\otimes[\nu_2]) \uparrow [\nu]$ *induction coefficients* (IDC) of permutation groups, or the *outer–product reduction coefficients* (ORC). Expressed in terms of the generalized Young tableaux, (4-140) can be written as

$$|Y_m^{[\nu]\tau}(\omega^0)\rangle = \sum_{m_1 \omega_1 m_2 \omega_2} C^{[\nu]\tau,m}_{\nu_1 m_1 \omega_1, \nu_2 m_2 \omega_2} |Y_{m_1}^{[\nu_1]}(\omega_1)\rangle |Y_{m_2}^{[\nu_2]}(\omega_2)\rangle \ , \tag{4-141}$$

where (ω^0) can be omitted. From (4-141), one gets

$$C^{[\nu]\tau,m}_{\nu_1 m_1 \omega_1, \nu_2 m_2 \omega_2} = \langle Y_m^{[\nu]\tau} | Y_{m_1}^{[\nu_1]}(\omega_1) Y_{m_2}^{[\nu_2]}(\omega_2)\rangle \ . \tag{4-142}$$

From (4-28), (4-134) and (4-139) one obtains the eigenequations satisfied by the IDC,

$$\sum_{m_1' m_2' \omega'} \left[\langle m_1 m_2 \omega | C(f) | m_1' m_2' \omega'\rangle - \lambda_f \delta_{m_1 m_1'} \delta_{m_2 m_2'} \delta_{\omega\omega'}\right] C^{[\nu]\tau,m}_{\nu_1 m_1', \nu_2 m_2', \omega'} = 0 \ , \tag{4-143}$$

$$f = n, n-1, \ldots 2, \quad \tau = 1, 2, \ldots, \{\nu_1 \nu_2 \nu\} \ .$$

From (4-143) we can get both the outer–product reduction rule and the IDC.

According to (2-106h), the matrix element of the permutation R of S_n in the induced rep is

$$\langle m_1 m_2 \omega | R | m_1' m_2' \omega'\rangle = \mathcal{G}_{\omega\omega'}(R) D^{[\nu_1]}_{m_1 m_1'}(p_1) D^{[\nu_2]}_{m_2 m_2'}(p_2) \ , \tag{4-144a}$$

$$\mathcal{G}_{\omega\omega'}(R) = \begin{cases} 1\,, & \text{if } Q_\omega^{-1} R Q_{\omega'} = p_1 p_2 \in S_{n_1} \times S_{n_2} \\ 0\,, & \text{otherwise} \end{cases}\,, \tag{4-144b}$$

where $p_1 \in S_{n_1}$ and $p_2 \in S_{n_2}$. For example,

$$\langle m_1 m_2(146,235)|(46)|m_1' m_2'(134,256)\rangle = D^{[\nu_1]}_{m_1 m_1'}(23) D^{[\nu_2]}_{m_2 m_2'}(45)\,. \tag{4-145}$$

Having found the matrix elements of R, we can use (4-94) to calculate the matrix elements of $C(f)$ recursively. The matrices $\mathbf{C}(f)$ are real and symmetric. The IDC is obtained by diagonalizing the matrices $\mathbf{C}(n), \ldots \mathbf{C}(2)$ simultaneously.

Phase convention: The relative phase is determined by the Yamanouchi phase convention, while the overall phase is fixed by requiring that the IDC with $m_1 = m_2 = m = 1$ and with the smallest possible index ω be positive

$$C^{[\nu]\tau,1}_{[\nu_1]1,[\nu_2]1,\omega}|_{\omega_{\min}} > 0\,. \tag{4-146}$$

Example 1: Calculating the IDC of S_3 for $[2]\otimes[1]$. The products of the irreducible basis vectors of $S_2(12)$ and $S_3(3)$ are designated by

$$\varphi_1 = |\boxed{1\,2}\ \boxed{3}\rangle\,. \tag{4-147}$$

There are three normal order sequences: $(\omega) = (12, 3)$, $(13, 2)$ and $(23, 1)$. Thus $h_3 = 3$. The corresponding order–preserving permutations are $Q_\omega = e, (23), (123)$. Under the action of Q_ω, we have $N = h_{\nu_1} h_{\nu_2} h_3 = 1 \times 1 \times 3 = 3$ orthonormal vectors

$$|1\rangle = |\boxed{1\,2}\ \boxed{3}\rangle\,, \quad |2\rangle = |\boxed{1\,3}\ \boxed{2}\rangle\,, \quad |3\rangle = |\boxed{2\,3}\ \boxed{1}\rangle\,. \tag{4-148}$$

They carry the induced rep of S_3. From Table 4.15-1, it is easy to construct the matrix representatives of $C(2) = (12)$ and $C(3) = (12) + (23) + (13)$. A simultaneous diagonalization of $C(2)$ and $C(3)$ gives the IDC listed in Table 4.15-2.

Table 4.15-1. Action of the permutations on the vectors of (4-148).

φ_i \ p	(12)	(13)	(23)
1	1	3	2
2	3	2	1
3	2	1	3

Example 2: Calculating the IDC of S_4 for $[21]\otimes[1]$. The products of the irreducible basis vectors of $S_3(123)$ and $S_1(4)$ are

$$\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}\ \boxed{4}\right\rangle \text{ and } \left|\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}\ \boxed{4}\right\rangle\,. \tag{4-149a}$$

There are four normal order sequences (ω) which are listed in Table 4.15-2 along with their indices ω and parities δ_ω.

Under the operations of the $\binom{n}{n_1} = 4$ order–preserving permutations Q_ω, the basis vectors of (4-149a) give rise to eight orthonormal vectors φ_i listed in Table 4.15-3.

From this table we find the eigenfunctions of $C(2)$ are

$$\begin{aligned} &\lambda_2 = 1: \quad \psi_1 = \varphi_1\,,\ \psi_2 = \varphi_2\,,\ \psi_3 = \frac{1}{\sqrt{2}}(\varphi_3 + \varphi_4)\,,\ \psi_4 = \frac{1}{\sqrt{2}}(\varphi_7 + \varphi_8)\,, \\ &\lambda_2 = -1: \ \phi_1 = \frac{1}{\sqrt{2}}(\varphi_3 - \varphi_4)\,,\ \phi_2 = \varphi_5\,,\ \phi_3 = \varphi_6\,,\ \phi_4 = \frac{1}{\sqrt{2}}(\varphi_7 - \varphi_8)\,. \end{aligned} \tag{4-149b}$$

Table 4.15-2. Normal order sequence (ω).

$\omega(\delta_\omega)$	1(+)	2(−)	3(+)	4(−)
(ω)	(123, 4)	(124, 3)	(134, 2)	(234, 1)

Table 4.15-3. The basis $|m_1 m_2 \omega\rangle$ of the induced rep $([21]\otimes[1])\uparrow S_4$.

φ_0	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8
$m_1 m_2 \omega$	111	112	113	114	211	212	213	214
$Y^{[21]}_{m1}(\omega_1)Y^{[1]}(\omega_2)$	$\begin{array}{\|c\|c\|c\|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|c\|}\hline 1&2&3\\\hline 4\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|c\|}\hline 1&3&2\\\hline 4\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|c\|}\hline 2&3&1\\\hline 4\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|c\|}\hline 1&3&4\\\hline 2\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|c\|}\hline 1&4&3\\\hline 2\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|c\|}\hline 1&4&2\\\hline 3\\\cline{1-1}\end{array}$	$\begin{array}{\|c\|c\|c\|}\hline 2&4&1\\\hline 3\\\cline{1-1}\end{array}$

Using (4-144), (4-149), and the results of Ex. 2.8 we can also find the representations of $C(f)$ in the basis $\psi_1, \ldots, \psi_4$, denoted by $\mathbf{C}^{(+)}(f)$.

$$\mathbf{C}^{(+)}(4) = \begin{pmatrix} 0 & 1 & -\sqrt{\frac{1}{2}} & \sqrt{\frac{3}{2}} \\ 1 & 0 & \sqrt{2} & 0 \\ -\sqrt{\frac{1}{2}} & \sqrt{2} & 1 & 0 \\ \sqrt{\frac{3}{2}} & 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{C}^{(+)}(3) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & \sqrt{2} & 0 \\ 0 & \sqrt{2} & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{4-149c}$$

A simultaneous diagonalization of $\mathbf{C}^{(+)}(4)$ and $\mathbf{C}^{(+)}(3)$ gives the IDC with $\lambda_2 = +1$. Similarly, we can obtain the IDC with $\lambda_2 = -1$ (see Table 4.17-3d).

The calculation of IDC by computer

The EFM for calculating the IDC can be easily implemented on a computer. The procedure of calculation is identical to that in Sec. 4.11. However the vector $\mathbf{U}^\tau$ in (4-112b) should be understood as the IDC, and (4-114) should be replaced by

$$C^{[\nu]\tau,m'}_{\nu_1 a,\nu_2 b,\omega} = \frac{1}{D^{[\nu]}_{m'm}(T)} \sum_{cd\omega'} [D^{[\nu_1]}_{ac}(p_1) D^{[\nu_2]}_{bd}(p_2) - D^{[\nu]}_{mm}(T)\delta_{ac}\delta_{bd}\delta_{\omega\omega'}] C^{[\nu]\tau,m}_{\nu_1 c,\nu_2 d,\omega'} . \tag{4-150}$$

Programs for calculating the IDC and the tables of IDC for S_3–S_6 are available (Chen, Wang, Lü, & Wu, 1987). The IDC of S_3–S_5 are listed in Table 4.17.

A much better algorithm for the IDC will be discussed in Sec. 7.17. That algorithm computes the IDC of S_n recursively.

4.16. Properties of the IDC

1. Unitarity

$$\begin{aligned} &\sum_{m_1 m_2 \omega} C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2,\omega} C^{[\nu]'\tau',m'}_{\nu_1 m_1,\nu_2 m_2,\omega} = \delta_{\nu\nu'}\delta_{\tau\tau'}\delta_{mm'} , \\ &\sum_{\nu\tau m} C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2,\omega} C^{[\nu]\tau,m}_{\nu_1 m'_1,\nu_2 m'_2,\omega'} = \delta_{m_1 m'_1}\delta_{m_2 m'_2}\delta_{\omega\omega'} . \end{aligned} \tag{4-151}$$

We can use (4-151b) to invert (4-139), giving

$$|m_1 m_2 \omega\rangle = \sum_{\nu\tau m} C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2,\omega} \Psi^{[\nu]\tau}_m . \tag{4-152}$$

2. Since $\{\nu_1\nu_2\nu\} = \{\nu_2\nu_1\nu\}$, we have

$$C^{[\nu]\tau,m}_{\nu_1 m\omega_1,\nu_2 m_2\omega_2} = \varepsilon_1 C^{[\nu]\tau,m}_{\nu_2 m_2\omega_2,\nu_1 m_1\omega_1} . \tag{4-153a}$$

The phase ε_1 is determined by the overall phase convention (4-146). Clearly

$$\varepsilon_1 = \mathrm{sign}\Big(C^{[\nu]\tau 1}_{[\nu_1]1,[\nu_2]1,\omega}|_{\omega_{\max}}\Big) \ . \tag{4-153b}$$

The values of ε_1 for S_2–S_5 are listed in Table A2 in the Appendix, and in Table 12 of Chen & Gao (1981).

It has been shown (Zhang & Li 1987) that for multiplicity free case the phase factor

$$\varepsilon_1 = (-1)^{[\nu_1]+[\nu_2]+[\nu]}, \tag{4-153c}$$

where the phase factor $(-1)^{[\nu]}$ can be calculated recursively by

$$(-1)^{[\nu]} = (-1)^{[\nu']+r_n+1}, \quad (-1)^{[1]} = 1, \tag{4-153d}$$

supposing that the Young diagram $[\nu]$ of S_n is obtained by adding a box to the row r_n of the Young diagram $[\nu']$ of S_{n-1}.

For the case $\nu_1 = \nu_2$ if the irrep ν occurs only once, then the IDC fulfill the following relation

$$C^{[\nu],m}_{\nu_1 m_1\omega_1,\nu_1 m_2\omega_2} = \delta_\nu C^{[\nu],m}_{\nu_1 m_2\omega_2,\nu_1 m_1\omega_1} \ , \tag{4-154a}$$

where $\delta_\nu = 1$ or -1. As in the case of the CG coefficients, we say that the representation with $\delta_\nu = 1$ (-1) belongs to the symmetric (anti-symmetric) product. If ν occurs more than once, then by taking appropriate linear combinations the IDC can be made to satisfy

$$C^{[\nu]\tau,m}_{\nu_1 m_1\omega_1,\nu_1 m_2\omega_2} = \delta_{\nu_\tau} C^{[\nu]\tau,m}_{\nu_1 m_2\omega_2,\nu_1 m_1\omega_1}, \quad \delta_{\nu_\tau} = \pm 1 \ . \tag{4-154b}$$

We will now derive an important property of the IDC. From (4-144a) and (4-67), we have

$$\langle \tilde{m}_1\tilde{m}_2\omega|R_a|\tilde{m}'_1\tilde{m}'_2\omega'\rangle = \delta_{p_1}\delta_{p_2}\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2}\Lambda^{\nu_1}_{m'_1}\Lambda^{\nu_2}_{m'_2}\langle m_1 m_2\omega|R_a|m'_1 m'_2\omega'\rangle \ , \tag{4-155}$$

where δ_{p_1} and δ_{p_2} are the parities of the permutations p_1 and p_2 determined from (4-144b). Putting $R = R_a$ in (4-144b) and equating the parities of both sides of (4-144b), we get

$$\delta_{p_1}\delta_{p_2} = \delta_a\delta_\omega\delta_{\omega'} \ .$$

Inserting this into (4-155), we find

$$\langle \tilde{m}_1\tilde{m}_2\omega|R_a|\tilde{m}'_1\tilde{m}'_2\omega'\rangle = \delta_a\delta_\omega\delta_{\omega'}\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2}\Lambda^{\nu_1}_{m'_1}\Lambda^{\nu_2}_{m'_2}\langle m_1 m_2\omega|R_a|m'_1 m'_2\omega\rangle \ . \tag{4-156a}$$

From (4-143) we have

$$\sum_{m'_1 m'_2\omega'} \langle \tilde{m}_1\tilde{m}_2\omega|C(f)|\tilde{m}'_1\tilde{m}'_2\omega'\rangle C^{[\tilde{\nu}]\tau,\tilde{m}}_{\tilde{\nu}_1\tilde{m}'_1,\tilde{\nu}_2\tilde{m}'_2,\omega'} = \lambda_f C^{[\tilde{\nu}]\tau,\tilde{m}}_{\tilde{\nu}_1\tilde{m}_1,\tilde{\nu}_2\tilde{m}_2,\omega}. \tag{4-156b}$$

Substituting (4-156a) into (4-156b), one obtains

$$\sum_{m'_1 m'_2\omega'} \langle m_1 m_2\omega|C(f)|m'_1 m'_2\omega'\rangle\delta_a\delta_\omega\delta_{\omega'}\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2}\Lambda^{\nu_1}_{m'_1}\Lambda^{\nu_2}_{m'_2}C^{[\tilde{\nu}]\tau,\tilde{m}}_{\tilde{\nu}_1\tilde{m}'_1,\tilde{\nu}_2\tilde{m}'_2,\omega'} = \lambda_f C^{[\tilde{\nu}]\tau,\tilde{m}}_{\tilde{\nu}_1\tilde{m}_1,\tilde{\nu}_2\tilde{m}_2,\omega} \ . \tag{4-156c}$$

Here $\delta_a = -1$ since $C(f)$ is a 2-cycle class operator. Furthermore, from (4-26a) we know that $\tilde{\lambda}_f = -\lambda_f$. Therefore (4-156c) can be rewritten as

$$\sum_{m'_1 m'_2\omega'} \langle m_1 m_2\omega|C(f)|m'_1 m'_2\omega'\rangle\delta_{\omega'}\Lambda^{\nu_1}_{m'_1}\Lambda^{\nu_2}_{m'_2}C^{[\tilde{\nu}]\tau,\tilde{m}}_{\tilde{\nu}_1\tilde{m}'_1,\tilde{\nu}_2\tilde{m}'_2,\omega'} = \tilde{\lambda}_f\delta_\omega\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2}C^{[\tilde{\nu}]\tau,\tilde{m}}_{\tilde{\nu}_1\tilde{m}_1,\tilde{\nu}_2\tilde{m}_2,\omega} \tag{4-157}$$

and we have

$$C^{(\tilde{\nu})\tau,\tilde{m}}_{\tilde{\nu}_1\tilde{m}_1,\tilde{\nu}_2\tilde{m}_2,\omega} = \eta^{\nu_\tau}_m \delta_\omega \Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2} \sum_{\tau'} a_{\tau\tau'} C^{[\nu]\tau',m}_{\nu_1 m_1,\nu_2 m_2,\omega} \ , \tag{4-158}$$

where $a_{\tau\tau'}$ are coefficients, and $\eta^{\nu_\tau}_m$ are phase factors. If ν_1, ν_2 and ν are not simultaneously self-conjugate, we can always choose the solution of the eigenequations so that

$$C^{(\tilde{\nu})\tau,\tilde{m}}_{\tilde{\nu}_1\tilde{m}_1,\tilde{\nu}_2\tilde{m}_2,\omega} = \eta^{\nu_\tau}_m \Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2} C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2,\omega} \ . \tag{4-159}$$

The phase factor $\eta^{\nu_\tau}_m$ can be determined in the following way. From (4-67) we have

$$\langle \Psi^{[\tilde{\nu}]\tau}_{\tilde{m}} | R_a | \Psi^{[\tilde{\nu}]\tau}_{\tilde{m}'} \rangle = \delta_a \Lambda^{\nu}_m \Lambda^{\nu}_{m'} \langle \Psi^{[\nu]\tau}_m | R_a | \Psi^{[\nu]\tau}_{m'} \rangle \ . \tag{4-160}$$

Using (4-156a) and (4-159) it follows that

$$\begin{aligned} \langle \Psi^{[\tilde{\nu}]\tau}_{\tilde{m}} | R_a | \Psi^{[\tilde{\nu}]\tau}_{\tilde{m}'} \rangle &= \eta^{\nu_\tau}_m \eta^{\nu_\tau}_{m'} \delta_a \sum C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2,\omega} C^{[\nu]\tau,m'}_{\nu_1 m'_1,\nu_2 m'_2,\omega'} \langle m_1 m_2 \omega | R_a | m'_1 m'_2 \omega' \rangle \\ &= \eta^{\nu_\tau}_m \eta^{\nu_\tau}_{m'} \delta_a \langle \Psi^{[\nu]\tau}_m | R_a | \Psi^{[\nu]\tau}_{m'} \rangle \ . \end{aligned} \tag{4-161a}$$

Comparing (4-160) with (4-161), we gather that

$$\eta^{\nu_\tau}_m = \varepsilon_2 \Lambda^{\nu}_m \ , \tag{4-161b}$$

where $\varepsilon_2 = \pm 1$ is dictated by the convention on the absolute phase of $\Psi^{[\nu]\tau}_m$. Inserting (4-161b) into (4-159), we arrive at an important symmetry of the IDC:

4.

$$C^{(\tilde{\nu})\tau,\tilde{m}}_{\tilde{\nu}_1\tilde{m}_1,\tilde{\nu}_2\tilde{m}_2,\omega} = \varepsilon_2 \delta_\omega \Lambda^{\nu}_m \Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2} C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2,\omega} \ , \tag{4-162a}$$

when ν_1, ν_2 and ν are not simultaneously self-conjugate. The phase factor ε_2 is again determined by the overall phase convention. Obviously

$$\varepsilon_2 = \Lambda^{\nu_1}_{h_{\nu_1}} \Lambda^{\nu_2}_{h_{\nu_2}} \Lambda^{\nu}_{h_\nu} \mathrm{sign}\big(\delta_\omega C^{[\nu]\tau,h_\nu}_{[\nu_1]h_{\nu_1},[\nu_2]h_{\nu_2},\omega}|_{\omega=\min}\big) \ . \tag{4-162b}$$

If ν_1, ν_2 and ν are simultaneously self-conjugate, then (4-162a) is replaced by

$$C^{[\nu]\tau,\tilde{m}}_{\nu_1\tilde{m}_1,\nu_2\tilde{m}_2,\omega} = \delta_\omega \Lambda^{\nu}_m \Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2} \sum_{\tau'} a_{\tau\tau'} C^{[\nu]\tau',m}_{\nu_1 m_1,\nu_2 m_2,\omega} \ . \tag{4-162c}$$

Equation (4-162a) shows that if $[\nu_1] \otimes [\nu_2] = \sum_\nu \{\nu_1\nu_2\nu\}[\nu]$, then $[\tilde{\nu}] \otimes [\tilde{\nu}_2] = \sum_\nu \{\nu_1\nu_2\nu\}[\tilde{\nu}]$, i.e., (4-138) holds.

It is worth mentioning some special cases. When $[\nu]$ is totally symmetric (in such cases $[\nu_1]$ and $[\nu_2]$ are necessarily also symmetric), the IDC is very simple

$$C^{[n],1}_{[n_1]1,[n_2]1,\omega} = \binom{n}{n_1}^{-\frac{1}{2}} \ . \tag{4-163a}$$

We obtain the IDC for the totally antisymmetric irrep from the symmetry in (4-162a),

$$C^{[1^n],1}_{[1^{n_1}]1,[1^{n_2}]1,\omega} = \delta_\omega \binom{n}{n_1}^{-\frac{1}{2}} \ . \tag{4-163b}$$

4.17. Tables of the IDC for S_3–S_5

Some remarks about the IDC tables are necessary.

1. In Tables 4.17-1 to 4.17-3, the generalized Young tableaux $Y^{\nu_1}_{m_1}(\omega_1)Y^{\nu_2}_{m_2}(\omega_2)$ are used as the table headings, while in Tables 4.17-4 to 4.17-8 the indices $(m_1 m_2 \omega)$ are used as the table headings. These two headings are interchangeable (see the example in Table 4.15-3).

2. The second column N is a normalization factor. The entries are the squares of the IDC. The asterisk denotes a negative IDC, and the blank denotes a zero IDC. Thus for instance, from Tables 4.17-5a, 5d and (4-142) we have

$$C^{[41],3}_{[21]2,[2]1,\omega=10} = \left\langle \begin{array}{|c|c|c|c|}\hline 1&2&4&5\\\hline 3\\\cline{1-1}\end{array} \;\middle|\; \begin{array}{|c|c|}\hline 3&5\\\hline 4\\\cline{1-1}\end{array}\;\begin{array}{|c|c|}\hline 1&2\\\hline\end{array} \right\rangle = -\sqrt{\frac{12}{180}} \ .$$

3. In Tables 4.17-3a, 3b, 4b, 5b, 5c, the tables for $[\nu_1] \otimes [\nu_2]$ and $[\tilde{\nu}_1] \otimes [\tilde{\nu}_2]$ are put together, one above and one below.

4. Each table may be read either horizontally or vertically.

5. Utilizing the symmetries (4-153) and (4-162), one can obtain IDC not listed in the tables. The necessary Λ^{ν}_{m} are listed in Table 4.4-1.

6. In the above discussion it is assumed that the single particle states in the Weyl tableau W_1 are entirely different from those in the tableau W_2. If this is not true, then we can prove that the basis

$$\Psi^{[\nu]\tau}_{m} = \sum_{m_1 m_2 \omega} C^{[\nu]\tau,m}_{\nu_1 m_1 \omega_1, \nu_2 m_2 \omega_2} \psi^{[\nu_1]}_{m_1}(\omega_1, W_1)\psi^{[\nu_2]}_{m_2}(\omega_2, W_2) \ , \tag{4-164a}$$

is still the Yamanouchi basis $[\nu]m$ of S_n (provided it is nonzero). However it is no longer normalized. We use the projection operator to prove this:

$$\begin{aligned} \Psi^{[\nu]\tau}_{m} &= \text{const } P^{[\nu]\overline{m}}_{m}\left[\psi^{[\nu_1]}_{\bar{m}_1}(\omega^0_1, W_1)\psi^{[\nu_2]}_{\bar{m}_2}(\omega^0_2, W_2)\right] \\ &= \sum_{m_1 m_2 \omega} C^{[\nu]\tau,m}_{\nu_1 m_1 \omega_1, \nu_2 m_2 \omega_2} \psi^{[\nu_1]}_{m_1}(\omega_1, W_1)\psi^{[\nu_2]}_{m_2}(\omega, W_2) \ . \end{aligned} \tag{4-164b}$$

Since the projection operator $P^{[\nu]\overline{m}}_{m}$ only affects the coordinate indices of $\psi^{[\nu_1]}_{m_1}$ and $\psi^{[\nu_2]}_{m_2}$, $\Psi^{[\nu]\tau}_{m}$ is the Yamanouchi basis $[\nu]m$ no matter whether the Weyl tableaux W_1 and W_2 have common single particle states or not.

As an example, suppose $\psi(12)$ and $\psi(34)$ are the orbital wave functions of two deuterons, with $[\nu_1] = [\nu_2] = [2]$. Using (4-164a) and Table 4.17-3b, and renormalizing the resulting functions, we obtain the Yamanouchi basis of S_4:

$$\begin{aligned} \Psi^{[4]} &= \sqrt{\frac{1}{3}}[\psi(12)\psi(34) + \psi(13)\psi(24) + \psi(14)\psi(23)] \ , \\ \Psi^{[22]}_{1} &= \sqrt{\frac{1}{6}}[2\psi(12)\psi(34) - \psi(13)\psi(24) - \psi(14)\psi(23)] \ , \\ \Psi^{[22]}_{2} &= \sqrt{\frac{1}{2}}[\psi(13)\psi(24) - \psi(14)\psi(23)] \ , \end{aligned} \tag{4-164c}$$

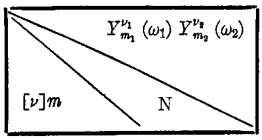
while the $\Psi^{[31]}_{m}$ are identically zero.

Table 4.17 The $([\nu_1] \otimes [\nu_2]) \uparrow [\nu]$ IDC of the permutation groups.

S_2 1 $[1]\otimes[1]=[2]\oplus[11]$

		1,2	2,1
[2]	2	1	1
[11]	2	1	*1

Table heading



S_3 2 $[2]\otimes[1]=[3]\oplus[21]$

		12,3;	13,2;	23,1
[3]	3	1	1	1
[21]1	6	4	*1	*1
2	2		1	*1
[21]1	2		1	1
2	6	4	1	*1
[1^3]	3	1	*1	1
		$\frac{1}{2},3$	$\frac{1}{3},2$	$\frac{2}{3},1$

$[11]\otimes[1]=[21]\oplus[1^3]$

S_4 3*a* $[3]\otimes[1]=[4]\oplus[31]$

		123,4;	124,3;	134,2;	234,1
[4]	4	1	1	1	1
[31]1	12	9	*1	*1	*1
2	6		4	*1	*1
3	2			1	*1
[211]1	2			1	1
2	6		4	1	*1
3	12	9	1	*1	1
[1^4]	4	1	*1	1	*1
		1	1	1	2
		2,4	2,3	3,2	3,1
		3	4	4	4

$[1^3]\otimes[1]=[211]\oplus[1^4]$

S_4 3*b* $[2]\otimes[2]=[4]\oplus[31]\oplus[22]$

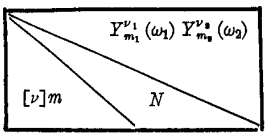
		12,34;	34,12;	23,14;	14,23;	13,24;	24,13
[4]	6	1	1	1	1	1	1
[31]1	6	1	*1	1	*1	1	*1
2	12	4	*4	*1	1	*1	1
3	4			*1	1	1	*1
[22]1	12	4	4	*1	*1	*1	*1
2	4			*1	*1	1	1
[22]1	4			1	1	1	1
2	12	4	4	*1	*1	1	1
[211]1	4			1	*1	1	*1
2	12	4	*4	*1	1	1	*1
3	6	*1	1	*1	1	1	*1
[1^4]	6	1	1	1	1	*1	*1
		1 3	3 1	2 1	1 2	1 2	2 1
		2,4	4,2	3,4	4,3	3,4	4,3

$[11]\otimes[11]=[22]+[211]+[1^4]$

cont'd

S_4 3c $[2]\otimes[11]=[31]\oplus[211]$

Table heading



		$12,\frac{3}{4}$;	$34,\frac{1}{2}$;	$23,\frac{1}{4}$;	$14,\frac{2}{3}$;	$13,\frac{2}{4}$;	$24,\frac{1}{3}$
[31]1	3	1		1		1	
2	24	*4		1	9	1	9
3	8		4	1	*1	*1	1
[211]1	8	4		*1	1	*1	1
2	24		4	*9	*1	9	1
3	3		1		1		*1

S_4 3d $[21]\otimes[1]=[31]\oplus[22]\oplus[211]$

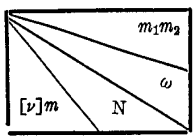
		$\frac{12}{3},4$;	$\frac{12}{4},3$;	$\frac{13}{4},2$;	$\frac{23}{4},1$	$\frac{13}{2},4$;	$\frac{14}{2},3$;	$\frac{14}{3},2$;	$\frac{24}{3},1$
[31]1	3		1	1	1				
2	96	36	4	*1	*1			27	27
3	32			1	*1	12	12	3	*3
[22]1	16	4	4	*1	*1			*3	*3
2	16			3	*3	4	*4	*1	1
[211]1	32	12	*12	3	3			*1	*1
2	96			*27	27	36	*4	*1	1
3	3						1	*1	1

S_5 4a $f_1=4$, $f_2=1$

$\omega(\delta\omega)$	1(+)	2(−)	3(+)	4(−)	5(+)
$(\omega)=(\omega_1,\ \omega_2)$	(1234, 5)	(1235, 4)	(1245, 3)	(1345, 2)	(2345, 1)

S_5 4b $[4]\otimes[1]=[5]\oplus[41]$

Table heading



		1,1				
		1	2	3	4	5
[5]	5	1	1	1	1	1
[41]1	20	16	*1	*1	*1	*1
2	12		9	*1	*1	*1
3	6			4	*1	*1
4	2				1	*1
[21^3]1	2				1	1
2	6			4	1	*1
3	12		9	1	*1	1
4	20	16	1	*1	1	*1
[1^5]	5	1	*1	1	*1	1

$[1^4]\otimes[1]=[21^3]\oplus[1^5]$

cont'd

S_5 4c $[31]\otimes[1]=[41]\oplus[32]\oplus[311]$

		1,1					2,1					3,1				
		1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
[41]1	4		1	1	1	1										
2	540	144	9	*1	*1	*1			128	128	128					
3	270			4	*1	*1	72	72	8	*2	*2				54	54
4	90				1	*1				2	*2	24	24	24	6	*6
[32]1	27	9	9	*1	*1	*1			*2	*2	*2					
2	432			128	*32	*32	144	*36	*4	1	1				*27	*27
3	144				32	*32				*1	1	48	*12	*12	*3	3
4	16							4	4	*1	*1				*3	*3
5	16									3	*3		4	*4	*1	1
[311]1	45	18	*18	2	2	2			*1	*1	*1					
2	1440			*512	128	128	576	*36	*4	1	1				*27	*27
3	480				*128	128				*1	1	192	*12	*12	*3	3
4	32							12	*12	3	3				*1	*1
5	96									*27	27		36	*4	*1	1
6	3													1	*1	1

S_5 4d $[211]\otimes[1]=[311]\oplus[221]\oplus[21^3]$

		1,1					2,1					3,1				
		1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
[311]1	3			1	1	1										
2	96		36	4	*1	*1				27	27					
3	32				1	*1		12	12	3	*3					
4	480	192	12	*12	3	3				*1	*1				128	128
5	1440				*27	27	576	36	*4	*1	1			512	128	*128
6	45								1	*1	1	18	18	2	*2	2
[221]1	16		4	4	*1	*1				*3	*3					
2	16				3	*3		4	*4	*1	1					
3	144	48	12	*12	3	3				*1	*1				*32	*32
4	432				*27	27	144	36	*4	*1	1			*128	*32	32
5	27								2	*2	2	9	*9	*1	1	*1
[21³]1	90	24	*24	24	*6	*6				2	2				*1	*1
2	270				54	*54	72	*72	8	2	*2			*4	*1	1
3	540								*128	128	*128	144	*9	*1	1	*1
4	4												1	*1	1	*1

cont'd

S_5 4e $[22]\otimes[1]=[32]\oplus[221]$

		1,1					2,1				
		1	2	3	4	5	1	2	3	4	5
[32]1	3			1	1	1					
2	96		36	4	*1	*1				27	27
3	32				1	*1		12	12	3	*3
4	32	16	4	4	*1	*1				*3	*3
5	32				3	*3	16	4	*4	*1	1
[221]1	32	16	*4	*4	1	1				3	3
2	32				*3	3	16	*4	4	1	*1
3	32		12	*12	3	3				*1	*1
4	96				*27	27		36	*4	*1	1
5	3								1	*1	1

S_5 5a $f_1=3, f_2=2$

ω $(\omega)=(\omega_1, \omega_2)$	1(+) (123,45)	2(−) (124,35)	3(+) (134,25)	4(−) (234,15)	5(+) (125,34)
ω $(\omega)=(\omega_1, \omega_2)$	6(−) (135,24)	7(+) (235,14)	8(+) (145,23)	9(−) (245,13)	10(+) (345,12)

S_5 5b $[3]\otimes[2]=[5]\oplus[41]\oplus[32]$

		1,1									
		1	2	3	4	5	6	7	8	9	10
[5]	10	1	1	1	1	1	1	1	1	1	1
[41]1	60	9	9	9	9	*4	*4	*4	*4	*4	*4
2	36	9	*1	*1	*1	4	4	4	*4	*4	*4
3	18		4	*1	*1	4	*1	*1	1	1	*4
4	6			1	*1		1	*1	1	*1	
[32]1	18	9	*1	*1	*1	*1	*1	*1	1	1	1
2	36		16	*4	*4	*4	1	1	*1	*1	4
3	12			4	*4		*1	1	*1	1	
4	12					4	*1	*1	*1	*1	4
5	4						1	*1	*1	1	
[221]1	4						1	1	1	1	
2	12					4	1	*1	*1	1	4
3	12			4	4		1	1	*1	*1	
4	36		16	4	*4	4	1	*1	1	*1	*4
5	18	9	1	*1	1	*1	1	*1	1	*1	1
[21³]1	6			1	1		*1	*1	1	1	
2	18		4	1	*1	*4	*1	1	*1	1	4
3	36	9	1	*1	1	4	*4	4	*4	4	*4
4	60	*9	9	*9	9	4	*4	4	4	*4	4
[1⁵]	10	1	*1	1	*1	1	*1	1	1	*1	1

$[1^3]\otimes[11]=[221]\oplus[21^3]\oplus[1^5]$

cont'd

S_5 5c $[3]\otimes[11]=[41]\oplus[311]$

		1,1									
		1	2	3	4	5	6	7	8	9	10
[41]1	4	1	1	1	1						
2	60	*9	1	1	1	16	16	16			
3	30		*4	1	1	*4	1	1	9	9	
4	10			*1	1		*1	1	*1	1	4
[311]1	15	9	*1	*1	*1	1	1	1			
2	120		64	*16	*16	*4	1	1	9	9	
3	40			16	*16		*1	1	*1	1	4
4	8					4	*1	*1	1	1	
5	24						9	*9	*1	1	4
6	3								1	*1	1
[311]1	3								1	1	1
2	24						9	9	1	1	*4
3	8					4	1	*1	1	*1	
4	40			16	16		1	1	*1	*1	4
5	120		64	16	*16	4	1	*1	*9	9	
6	15	9	1	*1	1	1	*1	1			
[21^3]1	10			1	1		*1	*1	1	1	*4
2	30		4	1	*1	*4	*1	1	9	*9	
3	60	9	1	*1	1	*16	16	*16			
4	4	1	*1	1	*1						

$[1^3]\otimes[2]=[311]\oplus[21^3]$

S_5 5d $[21]\otimes[2]=[41]\oplus[32]\oplus[311]\oplus[221]$

		1,1										2,1									
		1	2	3	4	5	6	7	8	9	10	1	2	3	4	5	6	7	8	9	10
[41]1	6					1	1	1	1	1	1										
2	90		16	16	16	1	1	1	*1	*1	*1								12	12	12
3	180	36	4	*1	*1	4	*1	*1	1	1	*4			27	27		27	27	3	3	*12
4	60			1	*1		1	*1	1	*1		12	12	3	*3	12	3	*3	3	*3	
[32]1	18		1	1	1	1	1	1	*1	*1	*1								*3	*3	*3
2	576	36	4	*1	*1	64	*16	*16	16	16	*64			27	27		*108	*108	*12	*12	48
3	192			1	*1		16	*16	16	*16		12	12	3	*3	*48	*12	12	*12	12	
4	192	36	36	*9	*9	16	*4	*4	*4	*4	16			*27	*27						
5	64			9	*9		4	*4	*4	4		12	*12	*3	3						
[311]1	30		3	3	3	*3	*3	*3	3	3	3								*1	*1	*1
2	960	108	12	*3	*3	*192	48	48	*48	*48	192			81	81		*36	*36	*4	*4	16
3	320			3	*3		*48	48	*48	48		36	36	9	*9	*16	*4	4	*4	4	
4	64	12	*12	3	3									*1	*1		4	4	*4	*4	16
5	192			*27	27							36	*4	*1	1	16	4	*4	*36	36	
6	6												1	*1	1	1	*1	1			
[221]1	64	4	4	*1	*1	*16	4	4	4	4	*16			*3	*3						
2	64			3	*3		*12	12	12	*12		4	*4	*1	1						
3	64	12	*12	3	3									*1	*1		*4	*4	4	4	*16
4	192			*27	27							36	*4	*1	1	*16	*4	4	36	*36	
5	6												1	*1	1	*1	1	*1			

cont'd

S_5 5e $[21]\otimes[11]=[32]\oplus[311]\oplus[221]\oplus[21^3]$

		1,1										2,1									
		1	2	3	4	5	6	7	8	9	10	1	2	3	4	5	6	7	8	9	10
[32]1	6		1	1	1	1	1	1													
2	192	36	4	*1	*1	*16	4	4	36	36				27	27						
3	64			1	*1		*4	4	*4	4	16	12	12	3	*3						
4	64	*4	*4	1	1									3	3		12	12	12	12	
5	64			*3	3							*4	4	1	*1	16	4	*4	*4	4	16
[311]1	6		1	1	1	*1	*1	*1													
2	192	36	4	*1	*1	16	*4	*4	*36	*36				27	27						
3	64			1	*1		4	*4	4	*4	*16	12	12	3	*3						
4	320	*36	36	*9	*9	16	*4	*4	4	4				3	3		48	48	*48	*48	
5	960			81	*81		36	*36	*4	4	16	*108	12	3	*3	192	48	*48	48	*48	*192
6	30								1	*1	1		*3	3	*3	*3	3	*3	3	*3	3
[221]1	64	12	12	*3	*3									*9	*9		4	4	4	4	
2	192			27	*27							36	*36	*9	9	16	4	*4	*4	4	16
3	192	*12	12	*3	*3	48	*12	*12	12	12				1	1		*16	*16	16	16	
4	576			27	*27		108	*108	*12	12	48	*36	4	1	*1	*64	*16	16	*16	16	64
5	18								3	*3	3		*1	1	*1	1	*1	1	*1	1	*1
[21³]1	60	12	*12	3	3	12	*3	*3	3	3				*1	*1		1	1	*1	*1	
2	180			*27	27		27	*27	*3	3	12	36	*4	*1	1	4	1	*1	1	*1	*4
3	90								12	*12	12		16	*16	16	*1	1	*1	1	*1	1
4	6															1	*1	1	1	*1	1

S_6 6a $f_1=5, f_2=1$

$\omega(\delta\omega)$ $(\omega)=(\omega_1, \omega_2)$	1(+) (12345, 6)	2(−) (12346, 5)	3(+) (12356, 4)	4(−) (12456, 3)	5(+) (13456, 2)	6(−) (23456, 1)

S_6 6b $[5]\otimes[1]=[6]\oplus[51]$

		1,1					
		1	2	3	4	5	6
[6]1	6	1	1	1	1	1	1
[51]1	30	25	*1	*1	*1	*1	*1
2	20		16	*1	*1	*1	*1
3	12			9	*1	*1	*1
4	6				4	*1	*1
5	2					1	*1

cont'd

S_6 7a $f_1=4, f_2=2$

$\omega(\delta\omega)$ $(\omega)=(\omega_1,\omega_2)$	1(+) (1234, 56)	2(−) (1235, 46)	3(+) (1245, 36)	4(−) (1345, 26)	5(+) (2345, 16)	6(+) (1236, 45)	7(−) (1246, 35)	8(+) (1346, 25)
	9(−) (2346, 15)	10(+) (1256, 34)	11(−) (1356, 24)	12(+) (2356, 14)	13(+) (1456, 23)	14(−) (2456, 13)	15(+) (3456, 12)	

S_6 7b $[4]\otimes[2]=[6]\oplus[51]\oplus[42]$

		1,1														
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
[6]	15	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
[51]1	30	4	4	4	4	4	*1	*1	*1	*1	*1	*1	*1	*1	*1	*1
2	80	16	*1	*1	*1	*1	9	9	9	9	*4	*4	*4	*4	*4	*4
3	48		9	*1	*1	*1	9	*1	*1	*1	4	4	4	*4	*4	*4
4	24			4	*1	*1		4	*1	*1	4	*1	*1	1	1	*4
5	8				1	*1			1	*1		1	*1	1	*1	
[42]1	240	144	*9	*9	*9	*9	*9	*9	*9	*9	4	4	4	4	4	4
2	144		81	*9	*9	*9	*9	1	1	1	*4	*4	*4	4	4	4
3	72			36	*9	*9		*4	1	1	*4	1	1	*1	*1	4
4	24				9	*9			*1	1		*1	1	*1	1	
5	18						9	*1	*1	*1	*1	*1	*1	1	1	1
6	36							16	*4	*4	*4	1	1	*1	*1	4
7	12								4	*4		*1	1	*1	1	
8	12										4	*1	*1	*1	*1	4
9	4											1	*1	*1	1	

S_6 8a $f_1=3, f_2=3$

$\omega(\delta\omega)$ $(\omega)=(\omega_1,\omega_2)$	1(+) (123, 456)	2(−) (124, 356)	3(+) (134, 256)	4(−) (234, 156)	5(+) (125, 346)	6(−) (135, 246)	7(+) (235, 146)	8(+) (145, 236)	9(−) (245, 136)	10(+) (345, 126)
	11(−) (126, 345)	12(+) (136, 245)	13(−) (236, 145)	14(−) (146, 235)	15(+) (246, 135)	16(−) (346, 125)	17(+) (156, 234)	18(−) (256, 134)	19(+) (356, 124)	20(−) (456, 123)

S_6 8b $[3]\otimes[3]=[6]\oplus[51]\oplus[42]\oplus[33]$

		1,1																			
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
[6]	20	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
[51]1	20	1	1	1	1	1	1	1	1	1	1	*1	*1	*1	*1	*1	*1	*1	*1	*1	*1
2	120	9	9	9	9	*4	*4	*4	*4	*4	*4	4	4	4	4	4	4	*9	*9	*9	*9
3	72	9	*1	*1	*1	4	4	4	*4	*4	*4	4	4	4	*4	*4	*4	1	1	1	*9
4	36		4	*1	*1	4	*1	*1	1	1	*4	4	*1	*1	1	1	*4	1	1	*4	
5	12			1	*1		1	*1	1	*1			1	*1	1	*1		1	*1		
[42]1	120	9	9	9	9	*4	*4	*4	*4	*4	*4	*4	*4	*4	*4	*4	*4	9	9	9	9
2	72	9	*1	*1	*1	4	4	4	*4	*4	*4	*4	*4	*4	4	4	4	*1	*1	*1	9
3	36		4	*1	*1	4	*1	*1	1	1	*4	*4	1	1	*1	*1	4	*1	*1	4	
4	12			1	*1		1	*1	1	*1			*1	1	*1	1		*1	1		
5	36	9	*1	*1	*1	*1	*1	*1	1	1	1	1	1	1	*1	*1	*1	*1	*1	*1	9
6	72		16	*4	*4	*4	1	1	*1	*1	4	4	*1	*1	1	1	*4	*4	*4	16	
7	24			4	*4		*1	1	*1	1			1	*1	1	*1		*4	4		
8	24					4	*1	*1	*1	*1	4	4	*1	*1	*1	*1	4				
9	8						1	*1	*1	1			1	*1	*1	1					
[33]1	36	9	*1	*1	*1	*1	*1	*1	1	1	1	*1	*1	*1	1	1	1	1	1	1	*9
2	72		16	*4	*4	*4	1	1	*1	*1	4	*4	1	1	*1	*1	4	4	4	*16	
3	24			4	*4		*1	1	*1	1			*1	1	*1	1		4	*4		
4	24					4	*1	*1	*1	*1	4	*4	1	1	1	1	*4				
5	8						1	*1	*1	1			*1	1	1	*1					

4.18. The $S_{n_1+n_2} \supset S_{n_1} \otimes S_{n_2}$ Irreducible Basis

4.18.1. The Frobenius reciprocity theorem and the $S_{n_1+n_2} \supset S_{n_1} \otimes S_{n_2}$ subduced basis

Before discussion the construction of the $S_{n_1+n_2} \supset S_{n_1} \otimes S_{n_2}$ subduced basis, we first cite the Frobenius reciprocity theorem

Frobenius reciprocity theorem: The number of times $\tau_\nu^{(\mu)}$ that an irrep ν of a group G occurs in the representation $D^{(\mu)} \uparrow G$ induced from an irrep μ of its subgroup G_s is equal to the number of times $\tau_\mu^{(\nu)}$ that the irrep μ of G_s appears in subduced representation $D^{(\nu)} \downarrow G_s$.

Proof: For simplicity, we use the notation $\bar{D}^{(\mu)}$ for the induced representation $D^{(\mu)} \uparrow G$. Due to (2-106f,g) the character $\bar{\chi}^{(\mu)}$ of the induced representation is

$$\begin{aligned}\bar{\chi}^{(\mu)}(R) &= \sum_\nu \tau_\nu^{(\mu)} \chi^{(\nu)}(R) \\ &= \sum_{i=1}^{q} \mathcal{G}_{ii}(R) \chi^{(\mu)}(a_i^{-1} R a_i) \ , \quad R \in G.\end{aligned}$$

Using (3-249b) we have

$$\tau_\nu^{(\mu)} = \frac{1}{|G|} \sum_R \sum_{i=1}^{q} \mathcal{G}_{ii}(R) \chi^{(\mu)}(a_i^{-1} R a_i) \chi^{(\nu)}(R)^* \ .$$

Due to (2-106h), on the right hand side we only need to sum over $R = a_i S a_i^{-1}$ $(S \in G_s)$. Note that $\chi^{(\nu)}(R) = \chi^{(\nu)}(S)$ and $|G| = q|G_s|$, we get

$$\tau_\nu^{(\mu)} = \frac{1}{|G_s|} \sum_S \chi^{(\mu)}(S) \chi^{(\nu)}(S)^* \ ,$$

which is just the coefficients $\tau_\mu^{(\nu)}$ in (2-106a). **QED**

An irrep $[\nu]$ of S_n is reducible with respect to its subgroup $S_{n_1} \otimes S_{n_2}, n_1 + n_2 = n$. The process of the reduction is known as subduction and is denoted by [see (2-106a)]

$$[\nu] \downarrow (S_{n_1} \otimes S_{n_2}) = \sum_\nu \{\nu_1 \nu_2 \nu\} ([\nu_1], [\nu_2]) \ . \tag{4-165a}$$

According to the Frobenius theorem, the multiplicities $\{\nu_1 \nu_2 \nu\}$ in (4-165a) and (4-135) are equal.

The subduced basis is written as $S_n \supset S_{n_1} \otimes S_{n_2}$ basis and has the basis functions

$$\left| \begin{matrix} [\nu] \\ \tau \nu_1 m_1 \nu_2 m_2 \end{matrix} \right\rangle \equiv \left| [\nu], \begin{matrix} \tau[\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \right\rangle \ , \quad \tau = 1, 2, \ldots, \{\nu_1 \nu_2 \nu\} \ . \tag{4-165b}$$

This basis belongs to the irrep $[\nu]$ of S_n, and at the same time is a Yamanouchi basis $[\nu_1]m_1$ for $S_{n_1} = S_{n_1}(1, 2, \ldots, n_1)$ and $[\nu_2]m_2$ for $S_{n_2} = S_{n_2}(n_1 + 1, \ldots, n)$.

The basis (4-165b) will be called the *non-standard basis* of S_n, it is used in many instances. The set of quantum numbers $(\tau[\nu_1]m_1[\nu_2]m_2)$ now serves as the component indices of the non-standard basis.

According to (3-265), the non-standard basis obeys the following eigenequations

$$\begin{pmatrix} C(n_1+n_2) \\ C(n_1) \\ C(s_1) \\ C'(n_2) \\ C'(s_2) \end{pmatrix} \left| [\nu], \begin{matrix} \tau[\nu_1] & [\nu_2] \\ m_1 & m_2 \end{matrix} \right\rangle = \begin{pmatrix} \nu \\ \nu_1 \\ m_1 \\ \nu_2 \\ m_2 \end{pmatrix} \left| [\nu], \begin{matrix} \tau[\nu_1] & [\nu_2] \\ m_1 & m_2 \end{matrix} \right\rangle \ , \tag{4-166}$$

$$(C'(n_2), C'(s_2)) = (C'(n_2), C'(n_2-1), \ldots, C'(2)) \ ,$$
$$C'(f) = \sum_{i>j=n_1+1}^{n_1+f} (ij), \quad f = n_2, n_2-1, \ldots 2 \ , \tag{4-167}$$

where $(C(n_1), C(s_1))$ is the CSCO-II of S_{n_1}, and $C(n_1+n_2)$ is the CSCO-I (instead of the 2-cycle class operator) of S_n.

Ex. 4.7. From the basis (4-32a), construct the $S_4 \supset S_2(12) \otimes S_2(34)$ basis.

4.18.2. Transformations between the standard basis and the non-standard bases of S_n

We usually expand the non-standard basis of S_n in terms of the standard basis of S_n,

$$\left| [\nu], \begin{matrix} \tau[\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \right\rangle = \sum_m \left| \begin{matrix} [\nu] \\ m \end{matrix} \right\rangle \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \right| [\nu], \begin{matrix} \tau[\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \Big\rangle \ , \tag{4-168a}$$

where the expansion coefficients are called the $[\nu] \downarrow ([\nu_1] \otimes [\nu_2])$ *subduction coefficients* (SDC) of S_n, or the transformation coefficients between the standard and non-standard basis of S_n.

Since the standard basis of S_n is also a standard basis of the subgroup S_{n_1}, the SDC is zero unless the tableau formed by the first n_1 numbers in $Y_m^{(\nu)}$ is identical to the Young tableau $Y_{m_1}^{(\nu_1)}$. Therefore the sum over m in (4-168a) is restricted to the Yamanouchi numbers $r_n, r_{n-1}, \ldots, r_{n_1+1}$. It follows that the SDC are independent of the quantum number m_1, while the partition $[\nu_1]$ is determined by $[\nu]m$ and the particle number n_2. Consequently, the SDC depends only on $[\nu], m, \tau, [\nu_2]$ and m_2 and its notation can be streamlined to

$$\left\langle \begin{matrix} [\nu] \\ m \end{matrix} \right| [\nu], \begin{matrix} \tau[\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \Big\rangle = \Big\langle [\nu] m | \tau, [\nu_2] m_2 \Big\rangle \ , \tag{4-169}$$

or expressed as

$$\left\langle \begin{matrix} [\nu] \\ m \end{matrix} \right| [\nu], \begin{matrix} \tau[\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \Big\rangle = \Big\langle Y_m^{[\nu]} | [\nu]\tau, Y_{m_1}^{[\nu_1]}(\omega_1^0) Y_{m_2}^{[\nu_2]}(\omega_2^0) \Big\rangle = \Big\langle Y_m^{[\nu]} | \tau, Y_{m_2}^{[\nu_2]}(\omega_2^0) \Big\rangle \ . \tag{4-170}$$

If the solutions of (4-166) are not unique for a given $\nu, \nu_1, m_1, \nu_2, m_2$, we must use the additional label τ to distinguish them. We may choose appropriate linear combinations so that the solutions with different τ are orthogonal. Consequently the non-standard basis (4-165b) forms an orthonormal complete set and the SDC fulfill the unitarity conditions

$$\sum_{\nu_2 m_2 \tau} \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \right| [\nu], \begin{matrix} \tau[\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \Big\rangle \left\langle \begin{matrix} [\nu] \\ m' \end{matrix} \right| [\nu], \begin{matrix} \tau[\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \Big\rangle = \delta_{mm'} \ , \tag{4-171a}$$

$$\sum_m \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \right| [\nu], \begin{matrix} \tau[\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \Big\rangle \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \right| [\nu], \begin{matrix} \tau'[\nu_1][\nu_2'] \\ m_1 m_2' \end{matrix} \Big\rangle = \delta_{\nu_2 \nu_2'} \delta_{m_2 m_2'} \delta_{\tau\tau'} \ . \tag{4-171b}$$

The inverse of (4-168a) is

$$\left| \begin{matrix} [\nu] \\ m \end{matrix} \right\rangle = \sum_{\nu_2 m_2 \tau} \left| [\nu], \begin{matrix} \tau[\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \right\rangle \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \right| [\nu], \begin{matrix} \tau[\nu_1][\nu_2] \\ m_1 m_2 \end{matrix} \Big\rangle \ . \tag{4-168b}$$

Another way of constructing the $S_n \supset S_{n_1} \otimes S_{n_2}$ basis is by means of the CG coefficients of the unitary group (see Sec. 7.18).

4.18.3. The calculation of the subduction coefficients (SDC)

The SDC is an important coefficient. In Secs. 7.14 and 7.15 we will see that the Racah coefficients and 9–ν coefficients of any SU_n group can be expressed in terms of them and in Sections 7.16 and 7.17 will show that the calculation of the $SU_{mn} \supset SU_m \times SU_n$ ISF and $SU_{m+n} \supset SU_m \otimes SU_n$ ISF also involves these coefficients. In the past, the rather cumbersome projection operator method was used to calculate the SDC (see Kaplan 1961). We can now use the following two methods to calculate them.

1. The *Eigenfunction method:* Each term on the right-hand side of (4-168a) is already an irreducible basis of S_n and S_{n_1}; therefore we only need to combine them into the standard basis $[\nu_2]m_2$ of S_{n_2}. In other words, to find the SDC we merely need to diagonalize the CSCO-II of S_{n_2} in the Yamanouchi basis $\left|\begin{matrix}[\nu]\\ m\end{matrix}\right\rangle$ with fixed $[\nu_1]m_1$:

$$\sum_{m'}\left[\left\langle\begin{matrix}[\nu]\\ m\end{matrix}\middle|\begin{matrix}C'(n_2)\\ C'(s_2)\end{matrix}\middle|\begin{matrix}[\nu]\\ m'\end{matrix}\right\rangle - \binom{\nu_2}{m_2}\delta_{mm'}\right]\left\langle\begin{matrix}[\nu]\\ m'\end{matrix}\middle|[\nu],\ \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle = 0\,. \tag{4-172}$$

In practical calculations, for a given set $[\nu],[\nu_1]$ and m_1(m_1 can be chosen arbitrarily, for example $m_1 = 1$), we construct the matrix representative of the CSCO-II $(C'(n_2), C'(s_2))$, or its variation $M = \sum_{f=2}^{n_2} k_f C'(f)$ (see (4-27a)], of S_{n_2} and diagonalize the matrices (or matrix). The eigenvectors are the required SDC. In order that the basis vectors $\left|[\nu],\ \begin{matrix}\tau[\nu_1]\,[\nu_2]\\ m_1\ \ m_2\end{matrix}\right\rangle$ with different m_2 have the correct phase, we again use (4-35). In this case it reads

$$\left|[\nu],\ \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2'\end{matrix}\right\rangle = \frac{1}{D^{[\nu_2]}_{m_2'm_2}(T_2')}\left[T - D^{[\nu_2]}_{m_2m_2}(T_2')\right]\left|[\nu],\ \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle,$$

$$T_2 = (i, i+1) \in S_{n_2}(n_1+1,\ldots,n_1+n_2);\quad T_2' = (i-n_1,\ i-n_1+1) \in S_{n_2}(1,2\ldots,n_2)\,. \tag{4-173}$$

From (4-173) we have

$$\left\langle\begin{matrix}[\nu]\\ m\end{matrix}\middle|[\nu],\ \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2'\end{matrix}\right\rangle = \frac{1}{D^{[\nu_2]}_{m_2'm_2}(T_2')}\sum_{m'}\left[D^{[\nu]}_{m'm}(T_2) - D^{[\nu_2]}_{m_2m_2}(T_2')\delta_{mm'}\right]\left\langle\begin{matrix}[\nu]\\ m'\end{matrix}\middle|[\nu],\ \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle. \tag{4-174}$$

It follows that for a given $[\nu],[\nu_1]$ and $[\nu_2]$ and starting with the SDC of the component m_2 we can obtain the SDC of other components m_2' with the correct relative phases by using (4-174). This algorithm can be easily realized on a computer.

2. *Using the IDC to find the SDC:*

Instead of using the projection operator $P^{[\nu]m'}_m$ we use the *generalized projection operator* (3-242a), or a shift operator from the non-standard basis to the standard basis of S_n,

$$\mathcal{P}^{[\nu],\tau[\nu_1]m_1'[\nu_2]m_2'}_m = \sqrt{\frac{h_\nu}{n!}}\sum_a\left\langle\begin{matrix}[\nu]\\ m\end{matrix}\middle|R_a\middle|[\nu],\ \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1'm_2'\end{matrix}\right\rangle R_a\,, \tag{4-175}$$

Making use of the left-coset decomposition (4-130), along with the following substitutions in (3-243a): $s_i \to Q_\omega, \Lambda\rho \to m, \bar{\Lambda}\bar{\rho} \to \tau[\nu_1]m_1'[\nu_2]m_2'$ we have the left-coset factored generalized projection operator

$$\mathcal{P}^{[\nu],\tau[\nu_1]m_1'[\nu_2]m_2'}_m = \sqrt{\frac{h_\nu}{h_{\nu_1}h_{\nu_2}}}\sqrt{\frac{n_1!n_2!}{n!}}\sum_{m_1m_2\omega}\left\langle\begin{matrix}[\nu]\\ m\end{matrix}\middle|Q_\omega\middle|[\nu],\ \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle Q_\omega P^{[\nu_1]m_1'}_{m_1}P^{[\nu_2]m_2'}_{m_2}\,. \tag{4-176a}$$

Applying (4-176a) to a normal order state $\Phi_0 = |i_1 i_2, \ldots i_n\rangle$ with n distinct single particle states, and using (3-225), we obtain

$$\begin{aligned}\Psi_m^{[\nu]\tau'} &= \mathcal{P}_m^{[\nu],\tau[\nu_1]m_1'[\nu_2]m_2'}\Phi_0 \\ &= \sqrt{\frac{h_\nu}{h_{\nu_1}h_{\nu_2}}}\sqrt{\frac{n_1!n_2!}{n!}}\sum_{m_1m_2\omega}\left\langle \begin{matrix}[\nu]\\ m\end{matrix}\middle| Q_\omega \middle| [\nu], \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle \psi_{m_1}^{[\nu_1]}(\omega_1)\psi_{m_2}^{[\nu_2]}(\omega_2)\ .\end{aligned} \tag{4-177}$$

The label τ' on the left-hand side of (4-177) is used to distinguish the different linearly independent functions $\Psi_m^{[\nu]\tau'}$ resulting from using different superscripts in the projection operator. We can choose $\tau' = \tau$, since τ' and τ have the same range and the choice of the additional label is arbitrary. Comparing (4-139) with (4-177), we obtain another expression for the IDC,

$$C^{[\nu]\tau,m}_{\nu_1m_1,\nu_2m_2,\omega} = \sqrt{\frac{h_\nu}{h_{\nu_1}h_{\nu_2}}}\sqrt{\frac{n_1!n_2!}{n!}}\left\langle \begin{matrix}[\nu]\\ m\end{matrix}\middle| Q_\omega \middle| [\nu], \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle . \tag{4-178a}$$

Letting $Q_\omega = e$ (identity), we obtain a relation between the SDC and the IDC,

$$\left\langle \begin{matrix}[\nu]\\ m\end{matrix}\middle| [\nu], \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle = \sqrt{\frac{h_{\nu_1}h_{\nu_2}}{h_\nu}}\sqrt{\frac{n!}{n_1!n_2!}}C^{[\nu]\tau,m}_{\nu_1m_1,\nu_2m_2,\omega^0}\ . \tag{4-179a}$$

Therefore once the IDC is known, the SDC can be found immediately, and vice versa.

The relation (4-178a) shows that the induction and subduction coefficients have the same multiplicity label τ, in confirming the Frobenius theorem. Moreover, this relation goes beyond the Frobenius reciprocity theorem; the latter only gives the relation between the multiplicities in the induction and subduction representation but not between the two coefficient.

Using (4-178a), the projection operator (4-176a) becomes (Horie 1964)

$$\mathcal{P}_m^{[\nu],\tau[\nu_1]m_1'[\nu_2]m_2'} = \sum_{m_1m_2\omega} C^{[\nu]\tau,m}_{\nu_1m_1,\nu_2m_2,\omega}Q_\omega P_{m_1}^{[\nu_1]m_1'}P_{m_2}^{[\nu_2]m_2'}\ . \tag{4-176b}$$

We can also define the transformation coefficients from the standard basis of S_n to the irreducible basis classified according to the group chain $S_n \supset S_{n_1}(\omega_1)\otimes S_{n_2}(\omega_2)$:

$$\left\langle \begin{matrix}[\nu]\\ m\end{matrix}\middle| [\nu], \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle_{(\omega)} = \left\langle Y_m^{[\nu]}\middle| [\nu]\tau,\ Y_{m_1}^{[\nu_1]}(\omega_1)Y_{m_2}^{[\nu_2]}(\omega_2)\right\rangle . \tag{4-178b}$$

From (4-178a) we have a relation between the generalized SDC and the IDC:

$$\left\langle \begin{matrix}[\nu]\\ m\end{matrix}\middle| [\nu], \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1m_2\end{matrix}\right\rangle_{(\omega)} = \sqrt{\frac{h_{\nu_1}h_{\nu_2}}{h_\nu}}\sqrt{\frac{n!}{n_1!n_2!}}C^{[\nu]\tau,m}_{\nu_1m_1,\nu_2m_2,\omega}\ . \tag{4-179b}$$

Note that according to (4-179a) the phase convention for IDC implies a phase convention for SDC:

$$\left\langle \begin{matrix}[\nu]\\ m\end{matrix}\middle| [\nu], \begin{matrix}\tau[\nu_1][\nu_2]\\ m_1\ \ 1\end{matrix}\right\rangle\Bigg|_{m=\min} > 0\ . \tag{4-179c}$$

The IDC symmetries (4-162a, c) together with $\delta_{\omega^0} = 1$ and (4-179a) allow us to obtain the following symmetries for SDC:

(i)

$$\left\langle \begin{matrix}[\tilde\nu]\\ \tilde m\end{matrix}\middle| [\tilde\nu], \begin{matrix}\tau\tilde\nu_1\tilde\nu_2\\ \tilde m_1\tilde m_2\end{matrix}\right\rangle = \varepsilon_3(\nu_1\nu_2\nu_\tau)\Lambda^\nu_m\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2}\left\langle \begin{matrix}[\nu]\\ m\end{matrix}\middle| [\nu], \begin{matrix}\tau\nu_1\nu_2\\ m_1m_2\end{matrix}\right\rangle , \tag{4-180a}$$

when ν_1, ν_2 and ν are not simultaneously self–conjugate.

(ii)

$$\left\langle \begin{matrix}[\nu] \\ \tilde{m}\end{matrix} \middle| [\nu], \begin{matrix}\tau\nu_1\nu_2 \\ \tilde{m}_1\tilde{m}_2\end{matrix} \right\rangle = \Lambda^{\nu}_{m}\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2}\sum_{\tau'} a_{\tau\tau'}\left\langle \begin{matrix}[\nu] \\ m\end{matrix} \middle| [\nu], \begin{matrix}\tau'\nu_1\nu_2 \\ m_1m_2\end{matrix} \right\rangle , \tag{4-180b}$$

when ν_1, ν_2 and ν are all self–conjugate. According to (4-179c) and (4-180a), we also have

$$\varepsilon_3(\nu'[1]\nu) = \Lambda^{\nu}_{\nu'},\ \varepsilon_3(\nu_1\nu_2\nu_\tau) = \mathrm{sign}\left(\Lambda^{\nu}_{m}\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{h_{\nu_2}} \left\langle \begin{matrix}[\nu] \\ m\end{matrix} \middle| [\nu], \begin{matrix}\tau[\nu_1][\nu_2] \\ m_1h_{\nu_2}\end{matrix} \right\rangle \Big|_{m=\min} \right) . \tag{4-180c}$$

Under Jahn's phase convention (see the footnote to Eq. (4-67)) (4-180a) simplifies to

$$\left\langle \begin{matrix}[\tilde{\nu}] \\ \tilde{m}\end{matrix} \middle| [\tilde{\nu}], \begin{matrix}\tau[\tilde{\nu}][\tilde{\nu}_2] \\ \tilde{m}_1\tilde{m}_2\end{matrix} \right\rangle = \varepsilon_3' \left\langle \begin{matrix}[\nu] \\ m\end{matrix} \middle| [\nu], \begin{matrix}\tau[\nu_1][\nu_2] \\ m_1m_2\end{matrix} \right\rangle . \tag{4-181}$$

3. *Special cases:* A number of cases now command our attention. (a) $n_2 = 1$.

$$\left\langle \begin{matrix}[\nu] \\ m\end{matrix} \middle| [\nu], \begin{matrix}[\nu_1][1] \\ m_1\end{matrix} \right\rangle = \delta_{(m)_1 m_1} , \tag{4-182a}$$

where $(m)_1$ is the Young tableau resulting from deleting the box with the number n in $Y^{[\nu]}_m$. (b) $n_2 = 2$.

The SDC for $n_2 = 2$ can be denoted simply by $\left\langle [\nu]m \middle| [\nu_2] \right\rangle$. (i) Suppose that n and $n-1$ are either in the same row or in the same column of the Young tableau $Y^{[\nu]}_m$; then

$$\left\langle \begin{matrix}[\nu] \\ m\end{matrix} \middle| [\nu], \begin{matrix}[\nu_1][\nu_2] \\ m_1\end{matrix} \right\rangle = \delta_{(m)_1 m} , \tag{4-182b}$$

where $(m)_1$ is the Young tableau resulting from deleting boxes with the numbers $n-1$ and n in $Y^{[\nu]}_m$. (ii) When $n-1$ and n are neither in the same row nor in the same column, from (4-166) and (4-14b) we know that to obtain the SDC one only needs to diagonalize the transposition $(n-1, n)$ in the 2–dimensional space with the basis vectors $|Y^{[\nu]}_m\rangle$ and $|Y^{[\nu]}_{m'}\rangle = |(n-1, n)Y^{[\nu]}_m\rangle$. Assuming that the Yamanouchi symbol m is larger than m', from (4-17) we obtain the matrix representative of $(n-1, n)$ in the space $\{Y^{[\nu]}_m, Y^{[\nu]}_{m'}\}$,

$$\mathcal{D}(n, n-1) = \begin{pmatrix} -\frac{1}{\sigma} & \frac{\sqrt{\sigma^2-1}}{\sigma} \\ \frac{\sqrt{\sigma^2-1}}{\sigma} & \frac{1}{\sigma} \end{pmatrix} , \quad \begin{matrix} \begin{array}{|c|c|c|c|}\hline & & & n' \\ \hline n \\ \cline{1-1} \end{array} & Y^{[\nu]}_m , \\ \begin{array}{|c|c|c|c|}\hline & & & n \\ \hline n' \\ \cline{1-1} \end{array} & Y^{[\nu]}_{m'} , \end{matrix} \quad n' = n-1 , \tag{4-183}$$

where σ is the axial distance from $n-1$ to n in $Y^{[\nu]}_{m'}, \sigma > 0$. A diagonalization of (4-183) gives the SDC listed below:

The SDC $\langle [\nu]\ \mathrm{m} \big| [\nu_2] \rangle$, $[\nu_2]$=[2],[11].

	[2]	[11]
$[\nu]m$	$\left(\frac{\sigma-1}{2\sigma}\right)^{1/2}$	$\left(\frac{\sigma+1}{2\sigma}\right)^{1/2}$
$[\nu]m'$	$\left(\frac{\sigma+1}{2\sigma}\right)^{1/2}$	$-\left(\frac{\sigma-1}{2\sigma}\right)^{1/2}$

(c) $n_2 = 3$. Analytic expressions for the $S_n \downarrow S_{n-3} \times S_3$ SDC have been found by McAven *et al.* (1998).

(d) From (4-179a) and (4-163), we get the SDC for the irreps $[n]$ and $[1^n]$;

$$\Big\langle [n] \big| [n]; [n_1][n_2] \Big\rangle = 1, \quad \Big\langle [1^n] \big| [1^n]; [1^{n_1}][1^{n_2}] \Big\rangle = 1 \,.$$

(e) Some SDC are trivial; for example

$$\left\langle \begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4&5\\\cline{1-2} 6\\\cline{1-1}\end{array} \middle| [321]; \begin{array}{|c|c|c|}\hline 1&2&3\\\hline\end{array} \begin{array}{|c|c|}\hline 4&5\\\hline 6\\\cline{1-1}\end{array} \right\rangle = 1 \,, \quad \left\langle \begin{array}{|c|c|c|}\hline 1&4&6\\\hline 2&5\\\cline{1-2} 3\\\cline{1-1}\end{array} \middle| [321]; \begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\cline{1-1}\end{array} \begin{array}{|c|c|}\hline 4&6\\\hline 5\\\cline{1-1}\end{array} \right\rangle = 1 \,. \qquad (4\text{-}185)$$

Algebraic expressions of the SDC have been given by Horie (1964) for the special case when $[\nu_1]$ and $[\nu_2]$ are totally symmetric, and by Li and Paldus (1990 [1]) when all irreps involved contain only two columns.

Tables 4.18-1 to 4.18-3 list the SDC for S_3–S_6. The trivial SDC such as those shown in (4-185) are omitted. N is the normalization factor. The entries are the squares of the SDC, with * designating a negative SDC. For instance, from Table 4.18-2a one has

$$\left\langle \begin{array}{|c|c|c|c|}\hline 1&2&4&5\\\hline 3\\\cline{1-1}\end{array} \middle| [41]; \begin{array}{|c|c|}\hline 1&2\\\hline\end{array} \begin{array}{|c|c|}\hline 3&4\\\hline 5\\\cline{1-1}\end{array} \right\rangle = \left\langle \begin{matrix}[41]\\3\end{matrix} \middle| [41]; \begin{matrix}[2]&[21]\\1&1\end{matrix} \right\rangle = -\sqrt{\frac{2}{18}}$$

Notice that the SDC for $[321]\downarrow ([21] \otimes [21])$ are not unique. The SDC in Table 4.18 3e(iv) satisfies the symmetry

$$\left\langle \begin{matrix}[321]\\ \tilde{m}\end{matrix} \middle| [321], \begin{matrix}\alpha[21][21]\\ \tilde{m}_1\tilde{m}_2\end{matrix} \right\rangle = \Lambda^{[321]}_{\tilde{m}} \Lambda^{[21]}_{\tilde{m}_1} \Lambda^{[21]}_{\tilde{m}_2} \left\langle \begin{matrix}[321]\\ m\end{matrix} \middle| [321], \begin{matrix}\beta[21][21]\\ m_1 m_2\end{matrix} \right\rangle .$$

A new and simpler method for the SDC, called the linear equation method, was proposed by Pan & Chen ([1] 1993).

4.18.4. Tables of the SDC for S_3–S_6

Table 4.18. The SDC for S_3–S_6.

1a $[\nu]=[31]$

$[\nu]m$ / $[\nu];\nu_1,\nu_2 m_2$	N	123 4	124 3	134 2
$[31];1,234$	9	1	2	6
$[31];1,\overset{23}{4}$	36	32	*1	*3
$1,\overset{24}{3}$	4		3	*1

1b $[\nu]=[22]$

	N	12 34	13 24
$[22];1,\overset{23}{4}$	4	1	3
$1,\overset{24}{3}$	4	3	*1

2b $[\nu]=[32]$

	N	123 45	124 35	134 25	125 34	135 24
$[32];1,\overset{234}{5}$	9	1	2	6		
$1,\overset{235}{4}$	144	32	*1	*3	27	81
$1,\overset{245}{3}$	16		3	*1	9	*3
$1,\overset{23}{45}$	48	32	*1	*3	*3	*9
$1,\overset{24}{35}$	16		9	*3	*3	1
$[32];12,345$	9	1	2		6	
$12,\overset{34}{5}$	9	2	4		*3	
$12,\overset{35}{4}$	3	2	*1			

2a $[\nu]=[41]$

	N	1234 5	1235 4	1245 3	1345 2
$[41];1,2345$	48	3	5	10	30
$1,\overset{234}{5}$	144	135	*1	*2	*6
$1,\overset{235}{4}$	36		32	*1	*3
$1,\overset{245}{3}$	4			3	*1
$[41];12,345$	18	3	5	10	
$12,\overset{34}{5}$	18	15	*1	*2	
$12,\overset{35}{4}$	3		2	*1	

2c $[\nu]=[311]$

m / $[\nu],\nu_1,\nu_2 m_2$	N	1	2	3	4	5	6
$[311];[1],[31]1$	9	1	2	6			
$[31]2$	576	*32	1	3	135	405	
$[31]3$	192		*9	3	*15	5	160
$[211]1$	192	160	*5	*15	3	9	
$[211]2$	576		*405	*135	*3	1	32
$[211]3$	9				6	*2	1
$[311];[2],[21]1$	3	1	2				
$[21]2$	18	*2	1		15		
$[1^3]$	18	10	*5		3		
$[11],[21]1$	18			15		*1	*2
$[21]2$	3					2	*1
$[3]$	18			3		5	10

cont'd

3a $[\nu]=[51]$

$[\nu], \nu_1, \nu_2 m_2$ \ m	N	1	2	3	4	5
[51]; [1][5]	50	2	3	5	10	30
[1][41]1	1200	1152	*3	*5	*10	*30
[41]2	144		135	*1	*2	*6
[41]3	36			32	*1	*3
[41]4	4				3	*1
[51]; [2][4]	20	2	3	5	10	
[2][31]1	180	162	*3	*5	*10	
[31]2	18		15	*1	*2	
[31]3	3			2	*1	
[51]; [3][3]	10	2	3	5		
[21]1	40	32	*3	*5		
[21]2	8		5	*3		

3b(i) $[\nu]=[42]$

	N	1	2	3	4	5	6	7	8	9
[42]; [1][41]1	48	3	5	10	30					
[41]2	1296	135	*1	*2	*6	128	256	768		
[41]3	324		32	*1	*3	64	*2	*6	54	162
[41]4	36			3	*1		6	*2	18	*6
[42]; [1][32]1	162	135	*1	*2	*6	*2	*4	*12		
[32]2	1296		1024	*32	*96	*32	1	3	*27	*81
[32]3	144			96	*32		*3	1	*9	3
[32]4	48					32	*1	*3	*3	*9
[32]5	16						9	*3	*3	1

3b(ii) $[\nu]=[42]$

$[\nu]\nu_1 m_1 \nu_2 m_2$ \ m	N	1	2	3	5	6	8
[42]; [2], [4]	108	3	5	10	10	20	60
[2][31]1	108	15	25	50	*2	*4	*12
[31]2	54	15	*1	*2	8	16	*12
[31]3	9		2	*1	4	*2	
[2][22]1	27	15	*1	*2	*2	*4	3
[22]2	9		4	*2	*2	1	
[42]; [3][3]	18	3	5		10		
[21]1	72	15	25		*32		
[21]2	8	5	*3				
[21]1[3]	9			1		2	6
[21]1	36			32		*1	*3
[21]2	4					3	*1

3c(i) $[\nu]=[411]$

		1	2	3	4	5	6	7	8	9	10
[411]; [1][41]1	48	3	5	10	30						
[41]2	3600	*135	1	2	6	384	768	2304			
[41]3	1800		*64	2	6	*96	3	9	405	1215	
[41]4	200			*6	2		*9	3	*15	5	160
[411]; [1][311]1	450	405	*3	*6	*18	2	4	12			
[311]2	14400		12288	*384	*1152	*32	1	3	135	405	
[311]3	4800			3456	*1152		*9	3	*15	5	160
[311]4	192					160	*5	*15	3	9	
[311]5	576						405	*135	*3	1	32
[311]6	9								6	*2	1

cont'd

3c(ii) $[\nu]=[411]$

	N	1	2	3	4	5	6	7	8	9	10
[411]; [2][31]1	18	3	5	10							
[31]2	180	*15	1	2		54	108				
[31]3	60		*4	2		*6	3		45		
[211]1	60	45	*3	*6		2	4				
[211]2	180		108	*54		*2	1		15		
[211]3	18					10	*5		3		
$[1^2][4]$	20				2			3		5	10
[31]1	180				162			*3		*5	*10
[31]2	18							15		*1	*2
[31]3	3									2	*1
[411]; [3][21]1	8	3	5								
[21]2	40	*5	3			32					
$[1^3]$	10	5	*3			2					
[21]1, [3]	10				2			3		5	
[21]1[21]1	40				32			*3		*5	
[21]2	8							5		*3	
[21]2, [3]	10					2			3		5
[21]1	40					32			*3		*5
[21]2	8								5		*3

3d $[\nu]=[33]$

	N	1	2	3	4	5
[33]; [1][32]1	9	1	2	6		
[32]2	144	32	*1	*3	27	81
[32]3	16		3	*1	9	*3
[32]4	48	32	*1	*3	*3	*9
[32]5	16		9	*3	*3	1
[2][31]1	9	1	2		6	
[31]2	9	2	4		*3	
[31]3	3	2	*1			
[21]1[21]1	4		1		3	
[21]2	4		3		*1	
[21]2, [21]1	4			1		3
[21]2	4			3		*1

3c(i) $[\nu]=[321]$, $n_1=1$, $n_2=5$

	N	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
[321]; [1][32]1	36	1	2	6			3	6	18								
[32]2	2304	128	*4	*12	108	324	*96	3	9	405	1215						
[32]3	256		12	*4	36	*12		*9	3	*15	5	160					
[32]4	768	*32	1	3	3	9							45	135	135	405	
[32]5	256		*9	3	3	*1							45	*15	*15	5	160
[1][311]1	36	3	6	18			*1	*2	*6								
[311]2	2304	384	*12	*36	324	972	32	*1	*3	*135	*405						
[311]3	768		108	*36	324	*108		9	*3	15	*5	*160					

3c(ii) $[\nu]=[321]$, $n_1=2$, $n_2=4$

	N	1	2	4	6	7	9	12	14
[321]; [2][31]1	9	1	2	6					
[31]2	576	*2	*4	3	54	108		405	
[31]3	192	*2	1		*6	3	45		135
[22]1	32	2	4	*3	6	12		*5	
[22]2	32	6	*3		*2	1	15		*5
[211]1	192	30	60	*45	*10	*20		27	
[211]2	576	270	*135		10	*5	*75		81
[211]3	18				10	*5	3		

cont'd

3e(iii) $[\nu]=[321]$, $n_1=2$, $n_2=4$

	N	3	5	8	10	11	13	15	16
[321]; [11][31]1	18	0	0	3	5	10	0	0	0
[31]2	576	81	0	75	*5	*10	0	135	270
[31]3	192	0	27	0	20	*10	45	60	*30
[22]1	32	5	0	15	*1	*2	0	*3	*6
[22]2	32	0	5	0	12	*6	*3	*4	2
[211]1	192	135	0	*45	3	6	0	*1	*2
[211]2	576	0	405	0	*108	54	*3	*4	2
[211]3	9	0	0	0	0	0	6	*2	1

3e(iv) $[\nu]=[321]$, $n_1=3$, $n_2=3$

m /	N	2	4	7	9	12	14	
[321]; [21]1[3]	32	1	3	3	5	5	15	[21]2[3]
[321]α; [21]1[21]1	64	9	27	3	5	*5	*15	α; [21]2, [21]1
[21]2	64	3	*1	25	*15	15	*5	[21]2
[321]β; [21]1[21]1	64	5	15	*15	*25	1	3	β; [21]2, [21]1
[21]2	64	*15	5	*5	3	27	*9	[21]2
[321]; [21]1[1^3]	32	15	*5	*5	3	3	*1	[21]2, [1^3]
	N	3	5	8	10	13	15	

Table 4.18-4. The phase factor ε_3 in Eq. (4-180a).

ν_1 ν_2 ν	ϵ_3	ν_1 ν_2 ν	ϵ_3	ν_1 ν_2 ν	ϵ_3	ν_1 ν_2 ν	ϵ_3
[1] [3] [31]	1	[1] [5] [51]	1	[3] [3] [42]	1	[3] [1^3] [411]	1
[1] [21]	1	[1] [41]	1	[3] [21]	−1	[21] [3]	1
[1] [4] [41]	−1	[2] [4]	−1	[21] [3]	1	[21] [21]	1
[1] [31]	1	[2] [31]	1	[21] [21]	1	[1] [32] [33]	1
[2] [3]	1	[3] [3]	1	[1] [41] [411]	−1	[2] [31]	−1
[2] [21]	1	[3] [21]	1	[1] [311]	1	[21] [21]	1
[1] [31] [32]	1	[1] [41] [42]	−1	[2] [31]	1		
[1] [22]	1	[1] [32]	1	[2] [221]	1		
[2] [3]	1	[2] [4]	1	[11] [4]	1		
[2] [21]	−1	[2] [31]	1	[11] [31]	−1		
		[2] [22]	1	[3] [21]	−1		

Ex. 4.8. Prove that

$$P_{m_1}^{[\nu_1]k_1} P_{m_2}^{[\nu_2]k_2} = \sum_{\nu m k \tau} \left(\frac{f_1! f_2! h_\nu}{f! h_{\nu_1} h_{\nu_2}}\right)^{\frac{1}{2}} \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \middle| [\nu], \begin{matrix} \tau\nu_1\nu_2 \\ m_1 m_2 \end{matrix} \right\rangle \left\langle \begin{matrix} [\nu] \\ k \end{matrix} \middle| [\nu], \begin{matrix} \tau\nu_1\nu_2 \\ k_1 k_2 \end{matrix} \right\rangle P_m^{[\nu]k} .$$

4.19. The $S_n \supset S_{n_1} \otimes S_{n_2}$ Isoscalar Factors*

4.19.1 The $S_n \supset S_{n-1}$ ISF

Let us first introduce some notation. The labelling of the irreducible bases of the three groups $S_n(x), S_n(\xi), S_n(q)$ and their subgroups $S_{n-1}(x), S_{n-1}(\xi), S_{n-1}(q)$ is listed in Table 4.19-1.

Table 4.19-1. Labelling of group and subgroup irreducible bases

$S_n(x)$	$S_{n-1}(x)$	$S_n(\xi)$	$S_{n-1}(\xi)$	$S_n(q)$	$S_{n-1}(q)$
$\left\vert \begin{matrix} [\sigma] \\ m_1 \end{matrix} \right\rangle = \left\vert \begin{matrix} \sigma \\ [\sigma']m_1' \end{matrix} \right\rangle$	$\left\vert \begin{matrix} [\sigma'] \\ m_1' \end{matrix} \right\rangle$	$\left\vert \begin{matrix} [\mu] \\ m_2 \end{matrix} \right\rangle = \left\vert \begin{matrix} [\mu] \\ [\mu']m_2' \end{matrix} \right\rangle$	$\left\vert \begin{matrix} [\mu'] \\ m_2' \end{matrix} \right\rangle$	$\left\vert \begin{matrix} [\nu] \\ m \end{matrix} \right\rangle = \left\vert \begin{matrix} [\nu] \\ [\nu']m' \end{matrix} \right\rangle$	$\left\vert \begin{matrix} [\nu'] \\ m' \end{matrix} \right\rangle$

Here m_1, m_1', m_2, and so on, can be understood either as the Young tableaux or the indices of the Young tableaux. From the branching law we have

$$[\sigma]m_1 = [\sigma][\sigma']m_1', \quad [\mu]m_2 = [\mu][\mu']m_2', \quad [\nu]m = [\nu][\nu']m' . \tag{4-186}$$

Let $Y_{m_1'}^{\sigma'}, Y_{m_2'}^{\mu'}$ and $Y_{m'}^{\nu'}$ be the Young tableaux after dropping the last box with the number n in the Young tableaux $Y_{m_1}^{\sigma}, Y_{m_2}^{\mu}$ and Y_m^{ν}, respectively. For example

$$\left\vert \begin{matrix} [42] \\ 9 \end{matrix} \right\rangle = \left\vert \begin{array}{|c|c|c|c|} \hline 1 & 3 & 5 & 6 \\ \hline 2 & 4 \\ \cline{1-2} \end{array} \right\rangle = \left\vert \begin{matrix} [42] \\ [32]5 \end{matrix} \right\rangle , \quad \left\vert \begin{matrix} [411] \\ 5 \end{matrix} \right\rangle = \left\vert \begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 6 \\ \hline 4 \\ \cline{1-1} 5 \\ \cline{1-1} \end{array} \right\rangle = \left\vert \begin{matrix} [411] \\ [311]1 \end{matrix} \right\rangle .$$

To construct irreducible basis vectors of $S_n(q)$, we first use the CG coefficients $C_{\sigma' m_1', \mu' m_2'}^{[\nu']\beta', m'}$ of S_{n-1} to combine linearly the products of the irreducible basis vectors of $S_n(x)$ and $S_n(\xi)$ into the irreducible basis $[\nu']m'$ of $S_{n-1}(q)$, that is,

$$|(\sigma'\mu')\beta'\rangle \equiv \left[\left\vert \begin{matrix} [\sigma] \\ [\sigma'] \end{matrix} \right\rangle \left\vert \begin{matrix} [\mu] \\ [\mu'] \end{matrix} \right\rangle \right]_{m'}^{[\nu']\beta'} \equiv \sum_{m_1' m_2'} C_{\sigma' m_1', \mu' m_2'}^{[\nu']\beta', m'} \left\vert \begin{matrix} [\sigma] \\ [\sigma']m_1' \end{matrix} \right\rangle \left\vert \begin{matrix} [\mu] \\ [\mu']m_2' \end{matrix} \right\rangle , \tag{4-187}$$

and then employ the $S_n \supset S_{n-1}$ ISF $C_{\sigma\sigma', \mu\mu'}^{[\nu]\beta, [\nu']\beta'}$ to combine (4-187) into the irreducible basis $[\nu]m$ of $S_n(q)$,

$$\left\vert \begin{matrix} [\nu]\beta \\ m \end{matrix} \right\rangle = \left\vert \begin{matrix} [\nu]\beta \\ [\nu']m' \end{matrix} \right\rangle = \sum_{\sigma'\mu'\beta'} C_{\sigma\sigma', \mu\mu'}^{[\nu]\beta, [\nu']\beta'} \left[\left\vert \begin{matrix} [\sigma] \\ [\sigma'] \end{matrix} \right\rangle \left\vert \begin{matrix} [\mu] \\ [\mu'] \end{matrix} \right\rangle \right]_{m'}^{[\nu']\beta'} . \tag{4-188}$$

Therefore the CG coefficients of S_n are expressed as [see (3-303)]

$$C_{[\sigma]m_1, [\mu]m_2}^{[\nu]\beta, m} = \sum_{\beta'} C_{\sigma\sigma, \mu\mu'}^{[\nu]\beta, [\nu']\beta'} C_{[\sigma']m_1', [\mu']m_2'}^{[\nu']\beta', m'} . \tag{4-189a}$$

For example we have

$$C_{[411]5, [411]7}^{[42]\beta, 9} = \sum_{\beta'} C_{[411][311], [411][311]}^{[42]\beta, [32]\beta'} C_{[311]1, [311]3}^{[32]\beta', 5} .$$

From (4-189a) we find

$$C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'} = \sum_{m'_1 m'_2} C^{[\nu]\beta,m}_{[\sigma]m_1,[\mu]m_2} C^{[\nu']\beta',m'}_{[\sigma']m'_1,[\mu']m'_2} \,. \tag{4-189b}$$

If the multiplicity label β' is redundant, we have from (4-189a) a simpler form for the ISF; namely,

$$C^{[\nu]\beta,[\nu']}_{\sigma\sigma',\mu\mu'} = C^{[\nu]\beta,m}_{[\sigma]m_1[\mu]m_2} / C^{[\nu']m'}_{[\sigma']m'_1,[\mu']m'_2} \,. \tag{4-189c}$$

The $S_n \supset S_{n-1}$ ISF satisfy the unitarity conditions (3-305) and (3-306). The inverse of (4-188) is

$$\left[\left| \begin{matrix} [\sigma] \\ [\sigma'] \end{matrix} \right\rangle \left| \begin{matrix} [\mu] \\ [\mu'] \end{matrix} \right\rangle \right]^{[\nu']\beta'}_{m'} = \sum_{\nu\beta} C^{[\nu]\beta[\nu']\beta'}_{\sigma\sigma',\mu\mu'} \left| \begin{matrix} [\nu]\beta \\ [\nu']m' \end{matrix} \right\rangle \,. \tag{4-190}$$

We now proceed to derive the eigenequation to be satisfied by the $S_n \supset S_{n-1}$ ISF. Since (4-188) is an eigenfunction of $C(n)$ and $C(n-1)$ with the eigenvalues ν and ν', respectively, we can use the relation $C(n) = C(n-1) + \sum_{i=1}^{n-1}(in)$ to obtain

$$\sum_{i=1}^{n-1}(in) \left| \begin{matrix} [\nu]\beta \\ [\nu']m' \end{matrix} \right\rangle = (\nu - \nu') \left| \begin{matrix} [\nu]\beta \\ [\nu']m' \end{matrix} \right\rangle \,. \tag{4-191}$$

Thus, to find the $S_n \supset S_{n-1}$ ISF, it suffices to diagonalize the operator $\sum_{i=1}^{n-1}(in)$ in the basis $|(\sigma'\mu')\beta'\rangle$ of (4-187), that is,

$$\sum_{\sigma'\mu'\beta'} \left[\sum_{i=1}^{n-1} \langle (\overline{\sigma}'\overline{\mu}')\overline{\beta}' | (in) | (\sigma'\mu')\beta' \rangle - (\nu - \nu')\delta_{\overline{\beta}'\beta'}\delta_{\overline{\sigma}'\sigma'}\delta_{\overline{\mu}'\mu'} \right] C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'} = 0 \,, \tag{4-192}$$

$$\beta = 1, 2, \ldots (\sigma\mu\nu), \quad \beta' = 1, 2, \ldots (\sigma'\mu'\nu') \,.$$

Since the matrix elements of $\Sigma_{i=1}^{n-1}(in)$ are independent of the quantum number m', we can use the identity $(in) = (i, n-1)(n-1, n)(i, n-1)$ and the orthonormality of the irreducible matrix elements to get

$$\begin{aligned} &\langle (\overline{\sigma}'\overline{\mu}')\overline{\beta}' | \sum_{i=1}^{n-1}(in) | (\sigma'\mu')\beta' \rangle \\ &= \frac{n-1}{h_{\nu'}} \sum_{\nu''} h_{\nu''} \langle (\overline{\sigma}', \overline{\mu}')\overline{\beta}' | (n-1, n) | (\sigma'\mu')\beta' \rangle \,, \end{aligned} \tag{4-193a}$$

where we used the branching law $m' = [\nu'']m''$. With the help of (4-187), the matrix elements of $(n-1, n)$ can be expressed in terms of the CG coefficients of S_{n-1} and the irreducible matrix elements of S_n:

$$\begin{aligned} &\langle (\overline{\sigma}'\overline{\mu}')\overline{\beta}' | (n-1, n) | (\sigma'\mu')\beta' \rangle \\ &= \sum_{\overline{m}'_1\overline{m}'_2 m'_1 m'_2} C^{[\nu']\overline{\beta}'m'}_{\overline{\sigma}'\overline{m}'_1,\overline{\mu}'\overline{m}'_2} C^{[\nu']\beta',m'}_{\sigma' m'_1,\mu' m'_2} D^{[\sigma]}_{\overline{m}_1 m_1}(n-1, n) D^{[\mu]}_{\overline{m}_2 m_2}(n-1, n) \,. \end{aligned} \tag{4-193b}$$

Since the dimension of the irreps of S_n increases very rapidly with n, (4-193b) is not suitable for computing the matrix element for large n. To simplify it we use the factorization (4-189a) for the S_{n-1} CG coefficients and obtain

$$\langle (\overline{\sigma}'\overline{\mu}')\overline{\beta}' | (n-1, n) | (\sigma'\mu')\beta' \rangle = M(\overline{\sigma}'\overline{\mu}'\overline{\beta}'\nu'\nu'', \sigma'\mu'\beta'\nu'\nu'') \,, \tag{4-193c}$$

$$M(\overline{\sigma}'\overline{\mu}'\overline{\beta}'\overline{\nu}'\nu'', \sigma'\mu'\beta'\nu'\nu'')$$
$$= \sum_{\sigma''\mu''\beta''} C^{[\overline{\nu}']\overline{\beta}',[\nu'']\beta''}_{\overline{\sigma}'\sigma'',\overline{\mu}\mu''} C^{[\nu']\beta',[\nu'']\beta''}_{\sigma'\sigma'',\mu'\mu''} D^{[\sigma]}_{\overline{\sigma}'\sigma'',\sigma'\sigma''}(n-1,n) D^{[\mu]}_{\overline{\mu}'\mu'',\mu'\mu''}(n-1,n) \ , \quad \text{(4-193d)}$$

where σ'', μ'' and ν'' refer to the group S_{n-2}. Notice that the right-hand side of (4-193c) is a special case ($\overline{\nu}' = \nu'$) of (4-193d). In Eq. (4-193d) only the $S_{n-1} \supset S_{n-2}$ ISF are involved instead of the S_{n-1} CG coefficients, and the summation runs only over $\sigma''\mu''\beta''$ instead of $\overline{m}'_1\overline{m}'_2 m'_1 m'_2$. Therefore the hurdle of the high dimensionality of the permutation group has been removed and we now can compute the $S_n \supset S_{n-1}$ ISF for much higher n than was previously possible. A program was written in Fortran-77 based on this algorithm (Novoselsky 1988).

For a given $[\sigma], [\mu]$ and $[\nu']$, we set up an eigenequation (4-192) of the order $l = \sum_{\sigma'\mu'}(\sigma'\mu'\nu')$. The order of the eigenequation (4-93) satisfied by the CG coefficients of S_n is equal to $L = h_\sigma h_\mu$ Notice that l is much smaller than L. For example, for $S_6, l_{\max} = 13$, while $L_{\max} = 256$. Therefore it is much easier to calculate the CG coefficients in terms of the ISF by using (4-189a) than to calculate the CG coefficients directly from (4-93).

The $S_n \supset S_{n-1}$ ISF is precisely the K coefficient defined by Hamermesh (1962) and Harvey (1981). A recursive formula for the K coefficient was given by Hamermesh.

Example 1: Use (4-189c) to find $S_5 \supset S_4$ ISF. From Table 4.13-3 we have

$$C^{[221],[22]}_{[41][4],[32][22]} = \left\langle \begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\hline 5\\\cline{1-1}\end{array} \middle| \begin{array}{|c|c|c|c|}\hline 1&2&3&4\\\hline 5\\\cline{1-1}\end{array} \begin{array}{|c|c|c|}\hline 1&2&5\\\hline 3&4\\\cline{1-2}\end{array} \right\rangle \Big/ \left\langle \begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\cline{1-2}\end{array} \middle| \begin{array}{|c|c|c|c|}\hline 1&2&3&4\\\hline\end{array} \begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\cline{1-2}\end{array} \right\rangle$$
$$= C^{[221],1}_{[41]1,[32]4} \Big/ C^{[22],1}_{[4]1,[22]1} = \sqrt{\tfrac{10}{16}} \Big/ 1 = \sqrt{\tfrac{5}{8}} \ .$$

Example 2: Find the $S_4 \supset S_3$ ISF $C^{[31],[21]}_{[31][\sigma'],[22][\mu']}$. According to the branching law, we know $[\sigma'] = [3]$, $[21]$ and $[\mu'] = [21]$. In solving (4-191), m' can take any permissible value. We put $m' = 1$ (the first component). Let

$$\varphi_1 = \left[\left| \begin{matrix}[31]\\[3]\end{matrix} \right\rangle \left| \begin{matrix}[22]\\[21]\end{matrix} \right\rangle \right]^{[21]}_1 = \left| \begin{matrix}1\,2\,3\\4\end{matrix} \right\rangle \left| \begin{matrix}1\,2\\3\,4\end{matrix} \right\rangle \ , \quad \text{(4-194a)}$$

$$\varphi_2 = \left[\left| \begin{matrix}[31]\\[21]\end{matrix} \right\rangle \left| \begin{matrix}[22]\\[21]\end{matrix} \right\rangle \right]^{[21]}_1 = -\sqrt{\tfrac{1}{2}} \left[\left| \begin{matrix}1\,2\,4\\3\end{matrix} \right\rangle \left| \begin{matrix}1\,2\\3\,4\end{matrix} \right\rangle - \left| \begin{matrix}1\,3\,4\\2\end{matrix} \right\rangle \left| \begin{matrix}1\,3\\2\,4\end{matrix} \right\rangle \right] \ . \quad \text{(4-194b)}$$

Here we used (4-187) and the S_3 CG coefficients, Table 4.13-1. With the help of the irreducible matrix elements of S_4 (Table 4.4-2), the representative of the operator [(14)+(24)+(32)] in the basis $\{\varphi_1, \varphi_2\}$ is $\left(\begin{smallmatrix}0 & 2\\ 2 & 0\end{smallmatrix}\right)$. Its eigenvalues are $\nu = 2, -2$, corresponding to [31] and [211]. Its eigenvectors are $\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$ and $\left(\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right)$. Therefore we have

$$\left| \begin{matrix}[31]\\[21]1\end{matrix} \right\rangle = \left| \begin{matrix}124\\3\end{matrix} \right\rangle = \tfrac{1}{\sqrt{2}}(\varphi_1 + \varphi_2) \ , \quad \left| \begin{matrix}[211]\\[21]1\end{matrix} \right\rangle = \left| \begin{matrix}1\,2\\3\\4\end{matrix} \right\rangle = \tfrac{1}{\sqrt{2}}(\varphi_1 - \varphi_2) \ . \quad \text{(4-194c)}$$

Substituting (4-194) into (4-194c), it is readily seen that the result is consistent with the CG coefficients of S_4 given in Table 4.13-2b.

In Sec. 7.16 it will be shown that the $S_n \supset S_{n-1}$ ISF is precisely the $SU_{mn} \supset SU_m \times SU_n$ ISF (or the single-particle CFP for the group chain $SU_{mn} \supset SU_m \times SU_n$).

4.19.2. Phase convention

1. Overall phase: The partitions are ordered according to their lengths. For example, for S_5, the partitions arranged in ascending order are [5], [41], [32], [311], [221], [21^3], and [1^5] and the partition [5] is said to be smaller than [41]. The pairs of partitions ($[\sigma'],[\mu']$) are ordered similarly. For the case of S_5, the order is: ([5],[5]), ([5],[41]),..., ([5],[1^5]), ([41],[5]), ([41],[41]),..., ([1^5],[1^5]). We demand that for a given $[\nu]$ and β, the first non-vanishing component of the vector $\{C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'}\}$ with the smallest $[\nu']$ be positive, the component of the vector being $\beta'\sigma'\mu'$.

It is easily recognized that this phase convention is consistent with the overall phase convention (4-146) of the CG coefficients.

2. Relative phase: By requiring that the relative phase be the Yamanouchi phase, we have from (4-188) and (4-193c) that

$$D^{[\nu]}_{\overline{m}m}(n-1,n) = \left\langle \begin{matrix}[\nu]\beta \\ \overline{m}\end{matrix} \middle| p_{nn-1} \middle| \begin{matrix}[\nu]\beta \\ m\end{matrix} \right\rangle = \sum_{\sigma'\mu'\beta'\overline{\sigma}'\overline{\mu}\overline{\beta}'} C^{(\nu)\beta,(\nu')\beta'}_{\sigma\sigma',\mu\mu'} \times C^{(\nu)\beta,(\overline{\nu}')\overline{\beta}'}_{\sigma\overline{\sigma}',\mu\overline{\mu}'} M(\overline{\sigma}'\overline{\mu}'\overline{\beta}'\overline{\nu}'\nu'',\sigma'\mu'\beta'\nu'\nu'') \ . \tag{4-195a}$$

Therefore

$$C^{(\nu)\beta,(\overline{\nu}')\overline{\beta}'}_{\sigma\overline{\sigma}',\mu\overline{\mu}'} = [D^{[\nu]}_{\overline{m}m}(n-1,n)]^{-1} \sum_{\sigma'\mu'\beta'} M(\overline{\sigma}'\overline{\mu}'\overline{\beta}'\overline{\nu}'\nu'',\sigma'\mu'\beta'\nu'\nu'') C^{(\nu)\beta,(\nu')\beta'}_{\sigma\sigma',\mu\mu'} \ , \tag{4-195b}$$

with $[\nu]\overline{m} = [\nu][\overline{\nu}'][\nu'']m''$ and $[\nu]m = [\nu][\nu'][\nu'']m''$. Eq. (4-195b) can be justified by multiplying both sides by $C^{(\nu)\beta,(\overline{\nu}')\overline{\beta}'}_{\sigma\overline{\sigma}',\mu\overline{\mu}'}$ and summing over $\overline{\sigma}'\overline{\mu}'\overline{\beta}'$.

Now the procedure for calculating the ISF can be described as follows: With σ and μ given for each $[\nu]$ and β we only need to get the ISF $C^{[\nu]\beta,(\nu')\beta'}_{\sigma\sigma'\mu\mu'}$ with the smallest ν' from the eigenequation (4-192) and the remaining ISF can be calculated from (4-195b). For a practical calculation of (4-195b), $\overline{m}'$ can be chosen as the first component, $\overline{m}' = 1$ and $\overline{m}$ is determined by $\overline{m}'$ and $\overline{\nu}'$ through $[\nu]\overline{m} = [\nu][\overline{\nu}']\overline{m}'$, while $[\nu]m$ is determined by $Y^{(\nu)}_m = (n-1,n)Y^{(\nu)}_{\overline{m}}$.

4.19.3. The properties of the $S_n \supset S_{n-1}$ ISF

1. The unitarity relations (3-305) and (3-306) now read as follows:

$$\begin{aligned} \sum_{\sigma'\mu'\beta'} C^{(\nu)\beta,(\nu')\beta'}_{\sigma\sigma',\mu\mu'} C^{(\overline{\nu})\overline{\beta},(\nu')\beta'}_{\sigma\sigma',\mu\mu'} &= \delta_{\nu\overline{\nu}}\delta_{\beta\overline{\beta}} \ , \\ \sum_{\nu\beta} C^{(\nu)\beta,(\nu')\beta'}_{\sigma\sigma',\mu\mu'} C^{(\nu)\beta,(\nu')\overline{\beta}'}_{\sigma\overline{\sigma}',\mu\overline{\mu}'} &= \delta_{\sigma'\overline{\sigma}'}\delta_{\mu'\overline{\mu}'}\delta_{\beta'\overline{\beta}'} \ . \end{aligned} \tag{4-196a}$$

Using (4-189) and the properties (4-116)-(4-123) of the CG coefficients, we obtain the following properties of the ISF (Gao & Chen 1985);

2.

$$C^{(\nu)\beta,(\nu')\beta'}_{\sigma\sigma',\mu\mu'} = \varepsilon'_1 C^{(\nu)\beta,(\nu')\beta'}_{\mu\mu',\sigma\sigma'} \tag{4-196b}$$

3.

$$\begin{aligned} \sqrt{\frac{h_{\nu'}}{h_\nu}} C^{(\nu)\beta,(\nu')\beta'}_{\sigma\sigma',\mu\mu'} &= \varepsilon'_2 \sqrt{\frac{h_{\sigma'}}{h_\sigma}} C^{(\sigma)\beta,(\sigma')\beta'}_{\nu\nu',\mu\mu'} \\ &= \varepsilon'_3 \sqrt{\frac{h_{\mu'}}{h_\mu}} C^{(\mu)\beta,(\mu')\beta'}_{\sigma\sigma',\nu\nu'} \ , \end{aligned} \tag{4-196c}$$

4.

$$\begin{aligned} C^{(\nu)\beta,(\nu')\beta'}_{\sigma\sigma',\mu\mu'} &= \varepsilon'_4 \Lambda^{\sigma}_{\sigma'} \Lambda^{\mu}_{\mu'} C^{(\nu)\beta,(\nu')\beta'}_{\tilde{\sigma}\tilde{\sigma}',\tilde{\mu}\tilde{\mu}'} \\ &= \varepsilon'_5 \Lambda^{\nu}_{\nu'} \Lambda^{\mu}_{\mu'} C^{(\tilde{\nu})\beta,(\tilde{\nu}')\beta'}_{\sigma\sigma',\tilde{\mu}\tilde{\mu}'} = \varepsilon'_6 \Lambda^{\sigma}_{\sigma'} \Lambda^{\nu}_{\nu'} C^{(\tilde{\nu})\beta,(\tilde{\nu}')\beta'}_{\tilde{\sigma}\tilde{\sigma}',\mu\mu'} \ , \end{aligned} \tag{4-196d}$$

where we used the factorization property of the phase factor (Butler 1979),

$$\Lambda^{\nu}_{m} = \Lambda^{\nu}_{\nu'}\Lambda^{\nu'}_{m'}, \quad \Lambda^{\nu}_{\nu'} = (-1)^{n_b} , \tag{4-196'}$$

where n_b is the number of boxes below the box labelled with n in the Young tableau Y^{ν}_{m} of S_n.

The phase factors ε'_i in the above equations can be expressed in terms of the phase factors ε_i appearing in the symmetries of the CG coefficients.

$$\varepsilon'_i = \varepsilon_i(\sigma\mu\nu_\beta)\varepsilon_i(\sigma'\mu'\nu'_{\beta'}), \quad i = 1, 2, \ldots, 6 . \tag{4-196e}$$

For the multiplicity-free case, the above symmetries are satisfied automatically. For the cases with multiplicities, we can choose the eigensolutions of (4-192) properly so that ISF fulfill these symmetries. Imposing these symmetries on the ISF leads to a partial, or sometimes even a total removal of the arbitrariness in the choice of the eigensolutions for the non-multiplicity-free case.

4.19.4. A special case

$$C^{[\nu],[\nu']}_{[n][n-1],[\mu][\mu']} = \delta_{\nu\mu}\delta_{\nu'\mu'}, \qquad C^{[\nu],[\nu']}_{[1^n][1^{n-1}],[\mu][\mu']} = \delta_{\nu\tilde{\mu}}\delta_{\nu'\tilde{\mu}'} , \tag{4-196f}$$

$$C^{[n][n-1]}_{[\sigma][\sigma'],[\mu][\mu']} = (h_{\sigma'}/h_\sigma)^{\frac{1}{2}}\delta_{\sigma\mu}\delta_{\sigma'\mu'}, \quad C^{[1^n][1^{n-1}]}_{[\sigma][\sigma'],[\mu][\mu']} = \Lambda^{\sigma}_{\sigma'}(h_{\sigma'}/h_\sigma)^{\frac{1}{2}}\delta_{\sigma\tilde{\mu}}\delta_{\sigma'\tilde{\mu}'} . \tag{4-196g}$$

Equation (4-196f) is obvious, while (4-196g) comes from (4-196f) and (4-196c).

4.19.5. Tables of the $S_n \supset S_{n-1}$ ISF

Here we list the $S_n \supset S_{n-1}$ ISF for $n \leq 5$. The $S_n \supset S_{n-1}$ ISF for $n \leq 6$ was given in Chen, Gao, Shi (1984).

The meaning of the heading is as follows:

$[\sigma][\mu]$	$[\nu']$
	$[\nu]_\beta$
$[\sigma'][\mu']$	

or

$[\sigma][\mu]$	$[\nu']$
	$[\nu]_\beta$
$[\sigma'][\mu']$	
$[\sigma'][\mu']$	
...	

for $\beta' > 1$

The trivial ISF which are obtainable from (4-196f) and (4-196g) are not included in the table. The tables are arranged in the order of $[\sigma], [\mu], [\nu']$. All the entries represent the square values of the ISF. A minus entry signifies a negative ISF.

Table 4.19. Tables of the $S_n \supset S_{n-1}$ ISF for n=3-5
(that is tables of the $SU_{mn} \supset SU_m \times SU_n$ single particle CFP for arbitrary m and n).

S_3: 1*a* [21]×[21]

[21][21]	[2]	
$\sigma'\mu'$ \ ν	[3]	[21]
[2][2]	1/2	1/2
[11][11]	1/2	−1/2

1*b*

[21][21]	[11]	
$\sigma'\mu'$ \ ν	[21]	[1³]
[2][11]	−1/2	1/2
[11][2]	−1/2	−1/2

S_4: 2*a* [31]×[31]

[31][31]	[3]	
	[4]	[31]
[3][3]	1/3	2/3
[21][21]	2/3	−1/3

2*b*

[31][31]	[21]		
	[31]	[22]	[211]
[3][21]	−1/6	1/3	1/2
[21][3]	−1/6	1/3	−1/2
[21][21]	2/3	1/3	

2*c*

[31][31]	[1⁴]
	[211]
[21][21]	1

3*a* [31]×[22]

[31][22]	[3]
	[31]
[21][21]	1

3*b*

[31][22]	[21]	
	[31]	[211]
[3][21]	1/2	1/2
[21][21]	1/2	−1/2

3*c*

[31][22]	[1³]
	[211]
[21][21]	−1

4*a* [31]×[211]

[31][211]	[3]
	[31]
[21][21]	1

4*b*

[31][211]	[21]		
	[31]	[22]	[211]
[3][21]	−1/2	1/3	1/6
[21][21]		−1/3	2/3
[21][1³]	1/2	1/3	1/6

4*c*

[31][211]	[1³]	
	[211]	[1⁴]
[3][1³]	−2/3	1/3
[21][21]	−1/3	−2/3

5*a* [22]×[22]

[22][22]	[3]
	[4]
[21][21]	1

5*b*

[22][22]	[21]
	[22]
[21][21]	1

5*c*

[22][22]	[1³]
	[1⁴]
[21][21]	1

6*a* [22]×[211]

[22][211]	[3]
	[31]
[21][21]	1

6*b*

[22][211]	[21]	
	[31]	[211]
[21][21]	−1/2	1/2
[21][1³]	−1/2	−1/2

6*c*

[22][211]	[1³]
	[211]
[21][21]	1

7*a* [211]×[211]

[211][211]	[3]	
	[4]	[31]
[21][21]	2/3	1/3
[1³][1³]	1/3	−2/3

cont'd

7b

[211][211]	[21]		
	[31]	[22]	[211]
[21][21]	2/3	1/3	
[21][1³]	−1/6	1/3	1/2
[1³][21]	−1/6	1/3	−1/2

7c

[211][211]	[1³]
	[211]
[21][21]	1

S_5: *8a* [41] × [41]

[41][41]	[4]	
	[5]	[41]
[4][4]	1/4	3/4
[31][31]	3/4	−1/4

8b

[41][41]	[31]		
	[41]	[32]	[311]
[4][31]	−1/12	5/12	1/2
[31][4]	−1/12	5/12	−1/2
[31][31]	5/6	1/6	

8c

[41][41]	[22]
	[32]
[31][31]	1

8d

[41][41]	[211]
	[311]
[31][31]	1

9a [41] × [32]

[41][32]	[4]
	[41]
[31][31]	1

9b

[41][32]	[31]		
	[41]	[32]	[311]
[4][31]	1/3	1/6	1/2
[31][31]	2/15	5/12	−9/20
[31][22]	8/15	−5/12	−1/20

9c

[41][32]	[22]	
	[32]	[221]
[4][22]	−3/8	5/8
[31][31]	−5/8	−3/8

9d

[41][32]	[211]	
	[311]	[221]
[31][31]	−1/4	3/4
[31][22]	3/4	1/4

10a [41] × [311]

[41][311]	[4]
	[41]
[31][31]	1

10b

[41][311]	[31]		
	[41]	[32]	[311]
[4][31]	−1/3	5/12	1/4
[31][31]		−3/8	5/8
[31][211]	2/3	5/24	1/8

10c

[41][311]	[22]	
	[32]	[221]
[31][31]	•1/16	15/16
[31][211]	15/16	1/16

10d

[41][311]	[211]		
	[311]	[221]	[21³]
[4][211]	−1/4	5/12	1/3
[31][31]	−1/8	5/24	−2/3
[31][211]	5/8	3/8	

10e

[41][311]	[1⁴]
	[21³]
[31][211]	1

cont'd

S_6: 11*a* [41] × [221]

[41][221]	[31]	
	[32]	[311]
[31][22]	1/4	3/4
[31][211]	3/4	−1/4

11*b*

[41][221]	[22]	
	[32]	[221]
[4][22]	−5/8	3/8
[31][211]	−3/8	−5/8

11*c*

[41][221]	[211]		
	[311]	[221]	[21^3]
[4][211]	1/2	−1/6	1/3
[31][22]	1/20	−5/12	−8/15
[31][211]	9/20	5/12	−2/15

11*d*

[41][221]	[1^6]
	[21^3]
[31][211]	−1

12*a* [41] × [21^3]

[41][21^3]	[31]
	[311]
[31][211]	1

12*b*

[41][21^3]	[22]
	[221]
[31][211]	1

12*c*

[41][21^3]	[211]		
	[311]	[221]	[21^3]
[4][211]	1/2	−5/12	1/12
[31][211]	0	1/6	5/6
[31][1^6]	1/2	5/12	−1/12

12*d*

[41][21^3]	[1^6]	
	[21^3]	[1^6]
[4][1^6]	−3/4	1/4
[31][211]	−1/4	−3/4

13*a* [32] × [32]

[32][32]	[4]	
	[5]	[41]
[31][31]	3/5	2/5
[22][22]	2/5	−3/5

13*b*

[32][32]	[31]		
	[41]	[32]	[311]
[31][31]	1/3	2/3	0
[31][22]	−1/3	1/6	1/2
[22][31]	−1/3	1/6	−1/2

13*c*

[32][32]	[22]	
	[32]	[221]
[31][31]	1/4	3/4
[22][22]	3/4	−1/4

13*d*

[32][32]	[211]		
	[311]	[221]	[21^3]
[31][31]	2/5	0	3/5
[31][22]	3/10	1/2	−1/5
[22][31]	−3/10	1/2	1/5

13*e*

[32][32]	[1^6]
	[21^3]
[22][22]	1

14*a* [32] × [311]

[32][311]	[4]
	[41]
[31][31]	1

14*b*

[32][311]	[31]			
	[41]	[32]	[311]α	[311]β
[31][31]	−3/10	0	3/5	1/10
[31][211]	−1/6	1/3	0	−1/2
[22][31]	−1/30	5/12	−3/20	2/5
[22][211]	1/2	1/4	1/4	0

cont'd

14c

[32][311]	[22]	
	[32]	[221]
[31][31]	−5/8	3/8
[31][211]	−3/8	−5/8

14d

[32][311]	[211]			
	[311]α	[311]β	[221]	[21^3]
[31][31]	0	1/2	−1/3	1/6
[31][211]	−3/5	1/10	0	−3/10
[22][31]	1/4	0	−1/4	−1/2
[22][211]	3/20	2/5	5/12	−1/30

14e

[32][311]	[1^4]
	[21^3]
[31][211]	1

15a [32] × [221]

[32][221]	[4]
	[41]
[22][22]	1

15b

[32][221]	[31]		
	[41]	[32]	[311]
[31][22]	−1/5	1/2	3/10
[31][211]	3/5	0	2/5
[22][211]	1/5	1/2	−3/10

15c

[32][221]	[22]	
	[32]	[221]
[31][211]	3/4	1/4
[22][22]	−1/4	3/4

15d

[32][221]	[211]		
	[311]	[221]	[21^3]
[31][22]	−1/2	1/6	1/3
[31][211]	0	2/3	−1/3
[22][211]	1/2	1/6	1/3

15e

[32][221]	[1^4]	
	[21^3]	[1^5]
[31][211]	−2/5	3/5
[22][22]	3/5	2/5

16a [32] × [21^3]

[32][21^3]	[31]	
	[32]	[311]
[31][211]	3/4	1/4
[22][211]	−1/4	3/4

16b

[32][21^3]	[22]	
	[32]	[221]
[31][211]	3/8	5/8
[22][1^4]	5/8	−3/8

16c

[32][21^3]	[211]		
	[311]	[221]	[21^3]
[31][211]	9/20	−5/12	2/15
[31][1^4]	−1/2	−1/6	1/3
[22][211]	1/20	5/12	8/15

16d

[32][21^3]	[1^4]
	[21^3]
[32][211]	1

17a [311] × [311]

[311][311]	[4]	
	[5]	[41]
[31][31]	1/2	1/2
[211][211]	1/2	−1/2

17b

[311][311]	[31]			
	[41]	[32]α	[32]β	[311]
[31][31]	5/12	1/2	1/12	0
[31][211]	−1/12	0	5/12	1/2
[211][31]	−1/12	0	5/12	−1/2
[211][211]	5/12	−1/2	1/12	0

17c

[311][311]	[22]			
	[32]α	[32]β	[221]α	[221]β
[31][31]	−3/16	1/2	5/16	0
[31][211]	5/16	0	3/16	1/2
[211][31]	5/16	0	3/16	−1/2
[211][211]	3/16	1/2	−5/16	0

cont'd

17*d*

[311][311]	[211]			
	[311]	[221]α	[221]β	[21^3]
[31][31]	1/2	0	−5/12	1/12
[31][211]	0	−1/2	1/12	5/12
[211][31]	0	−1/2	−1/12	−5/12
[211][211]	1/2	0	5/12	−1/12

17*e*

[311][311]	[1^4]	
	[21^2]	[1^5]
[31][211]	1/2	1/2
[211][31]	−1/2	1/2

18*a* [311] × [221]

[311][221]	[4]
	[41]
[211][211]	1

18*b*

[311][221]	[31]			
	[41]	[32]	[311]α	[311]β
[31][22]	1/2	1/4	1/4	0
[31][211]	1/6	−1/3	0	1/2
[211][22]	1/30	−5/12	3/20	−2/5
[211][211]	3/10	0	−3/5	−1/10

18*c*

[311][221]	[22]	
	[32]	[221]
[31][211]	−3/8	5/8
[211][211]	5/8	3/8

18*d*

[311][221]	[211]			
	[311]α	[311]β	[221]	[21^3]
[31][22]	3/20	2/5	−5/12	1/30
[31][211]	−3/5	1/10	0	3/10
[211][22]	−1/4	0	−1/4	−1/2
[211][211]	0	−1/2	−1/3	1/6

18*e*

[311][221]	[1^4]
	[21^2]
[31][211]	−1

19*a* [311] × [21^2]

[311][21^2]	[4]
	[41]
[211][211]	1

19*b*

[311][21^2]	[31]		
	[41]	[32]	[311]
[31][211]	−2/3	5/24	1/8
[211][211]	0	−3/8	5/8
[211][1^4]	1/3	5/12	1/4

19*c*

[311][21^2]	[32]	
	[32]	[221]
[31][211]	−15/16	1/16
[211][211]	−1/16	−15/16

19*d*

[311][21^2]	[211]		
	[311]	[221]	[21^3]
[31][211]	−5/8	3/8	0
[31][1^4]	−1/4	−5/12	1/3
[211][211]	−1/8	−5/24	−2/3

19*e*

[311][21^2]	[1^4]
	[21^2]
[31][211]	−1

20*a* [221] × [221]

[221][221]	[4]	
	[5]	[41]
[22][22]	2/5	3/5
[211][211]	3/5	−2/5

20*b*

[221][221]	[31]		
	[41]	[32]	[311]
[22][211]	−1/3	1/6	1/2
[211][22]	−1/3	1/6	−1/2
[211][211]	1/3	2/3	0

20c

[221][221]	[22]	
	[32]	[221]
[22][22]	3/4	1/4
[211][211]	1/4	−3/4

20d

[221][221]	[211]		
	[311]	[221]	[21³]
[22][211]	3/10	−1/2	1/5
[211][22]	−3/10	−1/2	−1/5
[211][211]	2/5	0	−3/5

20e

[221][221]	[1⁴]
	[21³]
[22][22]	−1

21a

[221][21³]	[4]
	[41]
[211][211]	1

21b

[221][21³]	[31]		
	[41]	[32]	[311]
[22][211]	−8/15	5/12	1/20
[211][211]	−2/15	−5/12	9/20
[211][1⁴]	−1/3	−1/6	−1/2

21c

[221][21³]	[22]	
	[32]	[221]
[22][1⁴]	3/8	5/8
[211][211]	5/8	−3/8

21d

[221][21³]	[211]	
	[311]	[221]
[22][211]	−3/4	1/4
[211][211]	1/4	3/4

22a [21³]×[21³]

[21³][21³]	[4]	
	[5]	[41]
[211][211]	3/4	1/4
[1⁴][1⁴]	1/4	−3/4

22b

[21³][21³]	[31]		
	[41]	[32]	[311]
[211][211]	5/6	1/6	0
[211][1⁴]	−1/12	5/12	1/2
[1⁴][211]	−1/12	5/12	−1/2

22c

[21³][21³]	[22]
	[32]
[211][211]	1

22d

[21³][21³]	[211]
	[311]
[211][211]	1

*4.19.6. The $S_{n_1+n_2} \supset S_{n_1} \otimes S_{n_2}$ ISF**

We introduce the following notation to denote the irreps of the nine groups:

$$\begin{pmatrix} \sigma' & \mu' & \nu' \\ \sigma'' & \mu'' & \nu'' \\ \sigma & \mu & \nu \end{pmatrix} , \begin{pmatrix} S_{n_1}(x) & S_{n_1}(\xi) & S_{n_1}(q) \\ S_{n_2}(x) & S_{n_2}(\xi) & S_{n_2}(q) \\ S_n(x) & S_n(\xi) & S_n(q) \end{pmatrix} . \tag{4-197}$$

For example, $[\mu'']$ and $[\sigma]$ are the irreps of $S_{n_2}(\xi)$ and $S_n(x)$, respectively, with $n = n_1 + n_2$. The $S_n \supset S_{n_1} \otimes S_{n_2}$ bases in the x, ξ and q spaces are denoted by

$$\left| \begin{matrix} [\sigma] \\ \theta[\sigma'][\sigma''][\sigma] m_1' m_1'' \end{matrix} \right\rangle , \quad \left| \begin{matrix} [\mu] \\ \varphi[\mu'][\mu''][\mu] m_2' m_2'' \end{matrix} \right\rangle , \quad \left| \begin{matrix} [\nu] \\ \tau[\nu'][\nu''][\nu] m' m'' \end{matrix} \right\rangle , \tag{4-198}$$

$$\theta = 1, 2, \ldots \{\sigma'\sigma''\sigma\}, \quad \varphi = 1, 2, \ldots \{\mu'\mu''\mu\}, \quad \tau = 1, 2, \ldots \{\nu'\nu''\nu\} .$$

The former two in (4-198) can be linearly combined into the third one via the following two steps:

1. Use the CG coefficients of S_{n_1} and S_{n_2} to combine them into the irreducible basis $[\nu']m'$ and $[\nu'']m''$ of $S_{n_1}(q)$ and $S_{n_2}(q)$, respectively,

$$\left|(\sigma'\sigma'')_\theta(\mu'\mu'')_\varphi\beta'\beta''\right\rangle = \left[\left|\begin{matrix}[\sigma]\\ \theta[\sigma'][\sigma'']\end{matrix}\right\rangle\left|\begin{matrix}[\mu]\\ \varphi[\mu'][\mu'']\end{matrix}\right\rangle\right]^{[\nu']_{\beta'}[\nu'']_{\beta''}}_{m'm''}$$

$$= \sum_{m_1'm_2'm_1''m_2''} C^{[\nu']\beta',m'}_{\sigma'm_1',\mu'm_2'} C^{[\nu'']\beta'',m''}_{\sigma''m_1'',\mu''m_2''} \left|\begin{matrix}[\sigma]\\ \theta[\sigma']m_1'[\sigma'']m_1''\end{matrix}\right\rangle\left|\begin{matrix}[\mu]\\ \varphi[\mu']m_2'[\mu'']m_2''\end{matrix}\right\rangle,$$

$$\beta' = 1,2,\ldots(\sigma'\mu'\nu'), \quad \beta'' = 1,2,\ldots(\sigma''\mu''\nu'') \ . \tag{4-199}$$

2. Use the $S_n \supset S_{n_1} \otimes S_{n_2}$ ISF to combine (4-199) into a basis belonging to the irrep $[\nu]$ of $S_n(q)$.

$$\left|\begin{matrix}[\nu]\beta\\ \tau[\nu']m'[\nu'']m''\end{matrix}\right\rangle = \sum_{\substack{\sigma'\sigma''\theta\beta'\\ \mu'\mu''\varphi\beta''}} C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\varphi\mu'\mu''} \left[\left|\begin{matrix}[\sigma]\\ \theta[\sigma'][\sigma'']\end{matrix}\right\rangle\left|\begin{matrix}[\mu]\\ \varphi[\mu'][\mu'']\end{matrix}\right\rangle\right]^{[\nu']_{\beta'}[\nu'']_{\beta''}}_{m'm''},$$

$$\beta = 1,2,\ldots(\sigma\mu\nu) \ . \tag{4-200}$$

The inverse of (4-200) is

$$\left[\left|\begin{matrix}[\sigma]\\ \theta[\sigma'][\sigma'']\end{matrix}\right\rangle\left|\begin{matrix}[\mu]\\ \varphi[\mu'][\mu'']\end{matrix}\right\rangle\right]^{[\nu']_{\beta'}[\nu'']_{\beta''}}_{m'm''} = \sum_{\nu\beta\tau} C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\varphi\mu'\mu''} \left|\begin{matrix}[\nu]\beta\\ \tau[\nu']m'[\nu'']m''\end{matrix}\right\rangle . \tag{4-201}$$

If a basis in the x–space is totally symmetric, then it is necessarily also a $S_n \supset S_{n_1} \otimes S_{n_2}$ irreducible basis, that is, $|[n]\rangle = \left|\begin{matrix}[n]\\ [n_1][n_2]\end{matrix}\right\rangle$. In such a special case we have:

$$\left|\begin{matrix}[\nu]\\ \tau[\nu']m'[\nu'']m''\end{matrix}\right\rangle^q = \delta_{\nu\mu}\delta_{\nu'\mu'}\delta_{\nu''\mu''}\delta_{\tau\varphi}\delta_{m'm_2'}\delta_{m''m_2''} \left|\begin{matrix}[n]\\ [n_1][n_2]\end{matrix}\right\rangle^x \left|\begin{matrix}[\mu]\\ \varphi[\mu']m_2'[\mu'']m_2''\end{matrix}\right\rangle^\xi . \tag{4-202}$$

Comparing this with (4-200), we have

$$C^{[\nu],\tau[\nu'][\nu'']}_{[n][n_1][n_2],[\mu]\varphi[\mu'][\mu'']} = \delta_{\nu\mu}\delta_{\nu'\mu'}\delta_{\nu''\mu''}\delta_{\tau\varphi} \ . \tag{4-203}$$

Analogously we have also

$$C^{[\nu],\tau[\nu'][\nu'']}_{[1^n][1^{n_1}][1^{n_2}],[\mu]\varphi\mu'\mu''} = \delta_{\nu\tilde{\mu}}\delta_{\nu'\tilde{\mu}'}\delta_{\nu''\tilde{\mu}''}\delta_{\tau\varphi} \ . \tag{4-204}$$

In Sec. 7.16 it will be proved that the $S_{n_1+n_2} \supset S_{n_1} \otimes S_{n_2}$ ISF is the n_2–particle CFP for the group chain $SU_{mn} \supset SU_m \times SU_n$.

4.20. Appendix: Derivation of Yamanouchi Matrix Elements by the EFM

In this section we use the ket $|\lambda\rangle = |\lambda_n\lambda_{n-1}\ldots\lambda_2\rangle$ to denote a Yamanouchi basis vector. From the relations

$$\big[(n-1,n), C(f)\big] = 0, \quad f = n, n-2, \ldots, 2 \ , \tag{4-205a}$$

$$\big[(n-1,n), C(n-1)\big] \neq 0 \ , \tag{4-205b}$$

we know that the permutation $(n-1,n)$ has non–vanishing matrix elements only between the states $|\lambda_n\lambda'_{n-1}\lambda_{n-2}\ldots\lambda_2\rangle$ and $|\lambda_n\lambda_{n-1}\lambda_{n-2}\ldots\lambda_2\rangle$, that is,

$$\langle\lambda'_n\lambda'_{n-1}\ldots\lambda'_2|(n-1,n)|\lambda_n\lambda_{n-1}\ldots\lambda_2\rangle = \text{const.}\ \delta_{\lambda'_n\lambda_n}\delta_{\lambda'_{n-2}\lambda_{n-2}}\ldots\delta_{\lambda'_2\lambda_2} \ . \tag{4-206}$$

We can easily establish the following identity relations

$$C(n) = C(n-1) + \sum_{i=1}^{n-1}(i,n) \ , \tag{4-207a}$$

$$\sum_{i=1}^{n-2}(i,n-1) = C(n-1) - C(n-2) \ , \tag{4-207b}$$

$$C(n) = C(n-1) + (n-1,n)\sum_{i=1}^{n-2}(i,n-1)(n-1,n) + (n-1,n) \ . \tag{4-207c}$$

Using (4-207b) and (4-205a), (4-207c) becomes

$$C(n) = C(n-1) - C(n-2) + (n-1,n)C(n-1)(n-1,n) + (n-1,n) \ , \tag{4-208a}$$

or written in a more elegant form

$$\big[C(n-1),(n-1,n)\big]_+ = \big(C(n) + C(n-2)\big)(n-1,n) - 1 \ , \tag{4-208b}$$

where $[A,B]_+ = AB + BA$.

Inserting (4-208b) between the two Yamanouchi basis vectors $|\lambda'\rangle$ and $|\lambda\rangle$ and using (4-28b) and (4-206), we obtain

$$\langle \lambda'_n\lambda'_{n-1}\dots\lambda'_2|(n-1,n)|\lambda_n\lambda_{n-1}\dots\lambda_2\rangle = \delta_{\lambda'_n\lambda_n}\delta_{\lambda'_{n-2}\lambda_{n-2}}\dots\delta_{\lambda'_2\lambda_2}\mu^{-1} \ , \tag{4-209}$$

$$\mu = \lambda_n - \lambda'_{n-1} - \lambda_{n-1} + \lambda_{n-2} \ .$$

From (4-209) we obtain the diagonal matrix element of the permutation $(n-1,n)$

$$\langle \lambda_n\lambda_{n-1}\dots\lambda_2|(n-1,n)|\lambda_n\lambda_{n-1}\dots\lambda_2\rangle = \sigma^{-1} \tag{4-210a}$$

$$\sigma = \lambda_n - 2\lambda_{n-1} + \lambda_{n-2} \tag{4-210b}$$

and the off-diagonal matrix elements

$$\langle \lambda_n\lambda'_{n-1}\dots\lambda_2|(n-1,n)|\lambda_n\lambda_{n-1}\dots\lambda_2\rangle = \begin{cases} 0, & \text{for } \mu \neq 0 \\ b, & \mu = 0 \end{cases} \ , \tag{4-211}$$

where the coefficient b is to be decided upon.

Before going on to consider the constant b, we first examine the conditions under which the permutation $(n-1,n)$ has non-vanishing off-diagonal matrix elements. Let $Y_{\lambda'}$ and Y_λ be the Young tableaux corresponding to the basis vectors $|\lambda_n\lambda'_{n-1}\lambda_{n-2}\dots\lambda_2\rangle$ and $|\lambda_n\lambda_{n-1}\lambda_{n-2}\dots\lambda_2\rangle$ which differ only in the second quantum number. Clearly, $Y_{\lambda'}$ and Y_λ must have the same Young diagrams $[\nu]$ and $[\nu'']$ for the numbers $1,\dots,n$ and $1,\dots n-2$, respectively. If the numbers n and $n-1$ are in the same row or column of the Young tableau Y_λ, the above condition implies that $Y_{\lambda'}$ and Y_λ must be identical. In other words, $(n-1,n)$ does not have non-vanishing matrix elements between two different states $|\lambda\rangle$ and $|\lambda'\rangle$ if one of them is symmetric or anti-symmetric in the indices $n-1$ and n. On the other hand, if n and $n-1$ are not at the same row or column of Y_λ, the above condition means that $Y_{\lambda'}$ and Y_λ differ only in the interchange of the positions of the numbers n and $n-1$.

Summarizing, only when n and $n-1$ are not in the same row or column of a Young tableau Y_λ, and only for a unique $Y_{\lambda'} = (n-1,n)Y_\lambda$, does the off-diagonal element $\langle\lambda'|(n-1,n)|\lambda\rangle$ differ from zero.

According to the identity $(n-1,n)^2 = 1$ and the above discussion, we immediately have

$$\langle\lambda|(n-1,n)|\lambda\rangle^2 + \langle\lambda|(n-1,n)|\lambda'\rangle\langle\lambda'|(n-1,n)|\lambda\rangle = 1\ . \tag{4-212}$$

Therefore the constant b is given by the equation

$$|b|^2 = 1 - 1/\sigma^2\ . \tag{4-213a}$$

Under the Yamanouchi phase convention, we have

$$\langle\lambda'|(n-1,n)|\lambda\rangle = \frac{\sqrt{\sigma^2-1}}{|\sigma|}\ . \tag{4-213b}$$

Finally, we are going to prove that the constant σ defined by (4-210b) is exactly the axial distance from $n-1$ to n in the Young tableau Y_λ.

Suppose that the row numbers of the indices n and $n-1$ in Y_λ are l and l', respectively. Then the row numbers of n and $n-1$ in Y'_λ are l' and l, respectively. It follows from (4-210b) and (4-3a) that

$$\begin{aligned}\sigma &= \frac{1}{2}\left[(f_l + f_{l'}) - 2(f_{l-1} + f_{l'}) + (f_{l-1} + f_{l'-1})\right] \\ &= \frac{1}{2}\left[(f_l - f_{l-1}) - (f_{l'} - f_{l'-1})\right]\ ,\end{aligned} \tag{4-214}$$

where

$$f_l = \nu_l(\nu_l - 2l)\ .$$

Therefore

$$\sigma = (\nu_l - l) - (\nu_{l'} - l')\ . \tag{4-215}$$

This is just the Eq. (4-16), since $\nu_l = c_n$, $\nu_{l'} = c_{n-1}, l = r_n$ and $l' = r_{n-1}$.

Chapter 5

Lie Groups

The theory of Lie groups and Lie algebras is so rich that here we are able only to cover a very small part of it here. Our main concerns are how to find the infinitesimal operators of the linear transformation groups, and how to generalize the new approach to the rep theory of finite groups to that of Lie groups, so that we can have a unified understanding of the rep theory of both finite groups and Lie groups. Using the concept of "representative of a vector" in quantum mechanics, the theorems on roots and weights are reformulated in a much more transparent way. In weight or root space, three representations, the Cartan, fundamental weight system, and simple root representations are discussed in great detail. Many theorems are cited without proof. Interested readers are referred to the books by Racah (1951), Wybourne (1974) and Bacry (1977).

5.1. Tensors

5.1.1. Vectors (rank one tensors)

We use superscripts and subscripts to denote the contravariant and covariant indices, respectively. Equations (2-7) and (2-8) are rewritten as

$$\mathbf{x} = x^{\mu}\ \mathbf{u}_{\mu}\ , \tag{5-1}$$

$$\mathbf{u}'_{\mu} = B_{\mu}{}^{\nu}\mathbf{u}_{\nu}, \quad x'^{\mu} = A^{\mu}{}_{\nu}x^{\nu}\ , \tag{5-2a, b}$$

where the dummy suffix summation convention is used. Notice that when A and B are written in matrix form, the superscript (subscript) of $A^{\mu}{}_{\nu}(B_{\mu}{}^{\nu})$ is the row index, i.e.,

$$A^{\mu}{}_{\nu} = A_{\mu\nu}, \quad B_{\mu}{}^{\nu} = B_{\mu\nu}, \quad B = \tilde{A}^{-1}\ . \tag{5-3}$$

For nonlinear transformations, contravariant and covariant coordinates are defined as those which satisfy the following relations:

$$dx'^{\mu} = A^{\mu}{}_{\nu}dx^{\nu}, \quad A^{\mu}{}_{\nu} = \frac{\partial x'^{\mu}}{\partial x^{\nu}}\ . \tag{5-4a, b}$$

$$dx'_{\mu} = B_{\mu}{}^{\nu}dx_{\nu}\ . \tag{5-5}$$

From (5-5) and (5-3) we have

$$\mathbf{u}_{\mu}dx^{\mu} = \mathbf{u}'_{\mu}dx'^{\mu} = \mathbf{u}_{\nu}B_{\mu}{}^{\nu}dx'^{\mu} = \mathbf{u}_{\nu}dx^{\nu}\ ;$$

therefore $dx^\nu = B_\mu{}^\nu dx'^\mu$ and

$$B_\mu{}^\nu = \frac{\partial x'_\mu}{\partial x_\nu} = \frac{\partial x^\nu}{\partial x'^\mu} \ . \tag{5-6}$$

Quantities which transform as dx^μ (dx_μ) are called contravariant (covariant) vectors, that is,

$$V'^\mu = A^\mu{}_\nu V^\nu, \quad V'_\mu = B_\mu{}^\nu V_\nu \ . \tag{5-7a, b}$$

It is easy to prove that the derivative of a scalar Φ with respect to the contravariant (covariant) variable is a covariant (contravariant) vector. For example,

$$\frac{\partial \Phi}{\partial x'^\mu} = \frac{\partial x^\nu}{\partial x'^\mu}\frac{\partial \Phi}{\partial x^\nu} = B_\mu{}^\nu \frac{\partial \Phi}{\partial x^\nu} \ . \tag{5-8}$$

Therefore the differential operators $\partial_\mu = \frac{\partial}{\partial x^\mu}$ and $\partial^\mu = \frac{\partial}{\partial x_\mu}$ can be regarded as covariant and contravariant vectors, respectively.

5.1.2. Tensors with rank higher than one

The tensors $T^{\mu\nu}, T_{\mu\nu}$ and T^μ_ν are called the contravariant, covariant, and mixed tensors of rank 2, respectively, if they satisfy the following transformation rules:

$$T'^{\mu\nu} = A^\mu{}_\rho A^\nu{}_\sigma T^{\rho\sigma}, \quad T'_{\mu\nu} = B_\mu{}^\rho B_\nu{}^\sigma T_{\rho\sigma} \ ,$$
$$T'^\mu{}_\nu = A^\mu{}_\rho B_\nu{}^\sigma T^\rho_\sigma \ . \tag{5-9a}$$

The above definition can be generalized to higher rank tensors. For example, there are mixed tensors of rank three which transform according to

$$T'^\tau{}_{\rho\sigma} = B_\rho{}^\mu B_\sigma{}^\nu A^\tau{}_\lambda T^\lambda_{\mu\nu} \ . \tag{5-9b}$$

5.1.3. The metric tensor

The metric tensor g_{ij} defined in (2-16) is a hermitian matrix. The scalar product of two vectors $\mathbf{x}$ and $\mathbf{y}$ in the space L is defined by

$$(\mathbf{x}, \mathbf{y}) = x^{\mu *} g_{\mu\nu} y^\nu \ . \tag{5-10}$$

This is a so-called *sesquilinear metric* (Gilmore, 1974). Another kind of metric is the *bilinear metric*, in which the scalar product is defined by

$$(\mathbf{x}, \mathbf{y}) = x^\mu g_{\mu\nu} y^\nu \ , \tag{5-11a}$$

and the metric tensor

$$g_{\mu\nu} = (\mathbf{u}_\mu, \mathbf{u}_\nu) \ , \tag{5-11b}$$

is a second-rank covariant tensor both for real and complex vector space. The inverse matrix of $(g_{\mu\nu})$ in such a metric is a second-rank contravariant tensor

$$g^{\sigma\nu} = (g^{-1})_{\nu\sigma} = M^{\sigma\nu}/\det(g_{\mu\nu}) \ , \tag{5-12a}$$

$$g_{\mu\nu} g^{\sigma\nu} = \delta^\sigma_\mu \ , \tag{5-12b}$$

where $M^{\sigma\nu}$ are the co-factors of the elements $g_{\sigma\nu}$ in the matrix g.

Using (5-12a), (2-111) becomes

$$|\overline{\varphi}_\sigma\rangle = |\varphi^\sigma\rangle = g^{\sigma\nu}|\varphi_\nu\rangle \ . \tag{5-12c}$$

Therefore the dual basis $|\overline{\varphi}_\sigma\rangle$ is a contravariant basis. Notice the difference between (5-10) and (5-11a), which disappears for real vectors.

5.1.4. Metric spaces

If in a space the contravariant and covariant vectors are obtainable from one another by the metric tensor, rather than being independent,

$$V_\mu = g_{\mu\nu}V^\nu, \quad V^\mu = g^{\mu\nu}V_\nu \ , \tag{5-13}$$

then the space is called a *metric space*. The relation above means the scalar product (5-11a) can be written as

$$(\mathbf{x},\mathbf{y}) = x^\mu y_\mu = x_\mu y^\mu \ . \tag{5-11c}$$

From (5-13) it is seen that the metric tensor can be used to raise or lower indices of vectors. This rule also holds for higher rank tensors, as for example

$$T^\nu_\mu = g_{\rho\mu}T^{\rho\nu} \ .$$

A summation over a pair of superscript and subscript is called a contraction, which reduces the rank of a tensor by two; for example, $U_{\nu\rho} = T^\mu_{\mu\nu\rho}(\equiv \sum_\mu T^\mu_{\mu\nu\rho})$ is a tensor of rank 2.

For orthonormal bases, $g_{\mu\nu} = \delta_{\mu\nu}$. Then (5-13) shows that $V^\mu = V_\mu$. In other words the covariant and contravariant vectors coincide for orthonormal bases.

From now on we will only deal with metric spaces.

Example: Consider the transformation from the Cartesian coordinates (x,y) to the polar coordinates (r,θ). For the Cartesian coordinates (x,y), the metric tensor is the unit matrix,

$$g = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \ , \tag{5-14}$$

and the covariant and contravariant are identical, that is, $dx^1 = dx_1 = dx, dx^2 = dx_2 = dy$. In the polar coordinate system, let r,θ be regarded as the contravariant coordinates, $dx'^1 = dr, dx'^2 = d\theta$. From $x = r\cos\theta, y = r\sin\theta$, we have

$$\begin{pmatrix} dx \\ dy \end{pmatrix} = \begin{pmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{pmatrix} \begin{pmatrix} dr \\ d\theta \end{pmatrix}, \quad A^{-1} = \begin{pmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{pmatrix} \ . \tag{5-15}$$

From A^{-1} we find

$$B = \tilde{A}^{-1} = \begin{pmatrix} \cos\theta & \sin\theta \\ -r\sin\theta & r\cos\theta \end{pmatrix} \ , \quad A = \begin{pmatrix} \cos\theta & \sin\theta \\ -\frac{1}{r}\sin\theta & \frac{1}{r}\cos\theta \end{pmatrix} \ . \tag{5-16}$$

From (5-9a), (5-14) and (5-16), we obtain the covariant metric tensor in the polar coordinate system:

$$(g'_{\mu\nu}) = g' = Bg\tilde{B} = \begin{pmatrix} 1 & 0 \\ 0 & r^2 \end{pmatrix} \ . \tag{5-17}$$

Moreover from (5-4a), (5-5) and (5-16) we have

$$\begin{pmatrix} dx'^1 \\ dx'^2 \end{pmatrix} = \begin{pmatrix} dr \\ d\theta \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\frac{\sin\theta}{r} & \frac{\cos\theta}{r} \end{pmatrix} \begin{pmatrix} dx \\ dy \end{pmatrix}, \quad \begin{pmatrix} dx'_1 \\ dx'_2 \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -r\sin\theta & r\cos\theta \end{pmatrix} \begin{pmatrix} dx \\ dy \end{pmatrix} \ . \tag{5-18}$$

It is easy to verify from (5-17) and (5-18) that

$$\begin{pmatrix} dx'_1 \\ dx'_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & r^2 \end{pmatrix} \begin{pmatrix} dx'^1 \\ dx'^2 \end{pmatrix} \ .$$

The invariant ds^2 is

$$ds^2 = dx^\mu g_{\mu\nu} dx^\nu = dx^2 + dy^2 = dx'^\mu g'_{\mu\nu} dx'^\nu = d^2r + r^2 d^2\theta \ .$$

5.2. Definition of a Lie Group; With Examples

A Lie group is a special kind of continuous group. The group elements $R(a)$ are labelled by r real parameters $a^1, a^2, \ldots, a^r$,

$$R(a) = R(a^1, a^2, \ldots, a^r) \ . \tag{5-19}$$

The parameters a^ρ may vary over a finite or an infinite range. The space of the r parameters is called the *group-parameter space.* A group G is called a Lie group of *order* r if $R(a)$ obeys the following five postulates:

1. The identity element $R(a_0)$ exists, that is,

$$R(a_0)R(a) = R(a)R(a_0) = R(a), \quad \text{for any } R(a) \in G \ . \tag{5-20}$$

The parameters a_0 of the identity element are usually taken as zero, that is, $R(a_0) = R(0)$.

2. For any a we can find $\bar{a}$ such that

$$R(\bar{a})R(a) = R(a)R(\bar{a}) = R(0) \ ,$$

i.e., for every $R(a)$ an inverse exists:

$$R(\bar{a}) = R^{-1}(a) \ . \tag{5-21}$$

3. For given parameters a and b, we can find c in the set of parameters such that

$$R(c) = R(b)R(a) \ , \tag{5-22}$$

where the parameters c are real functions of the real parameters a and b,

$$c = \varphi(a, b) \ . \tag{5-23}$$

Equation (5-23) is called the *combination law of group parameters* and tells us that the group is closed.

4. Associativity.

$$\begin{aligned} R(a)[R(b)R(c)] &= [R(a)R(b)]R(c) \ , \\ \varphi(\varphi(c, b), a) &= \varphi(c, \varphi(b, a)) \ . \end{aligned} \tag{5-24}$$

5. The parameters c in (5-23) are analytic functions of a and b, and the $\bar{a}$ in (5-21) are analytic functions of a.

A Lie group is said to be *compact* if its parameters are bounded.

Example 1: The real linear transformation group $GL(2, R)$ in two-dimensional space

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}, \quad R(a) = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \ . \tag{5-25}$$

The collection of all 2×2 nonsingular matrices $R(a)$ forms a real linear transformation group under matrix multiplication. Its elements are labelled by four real parameters $(a_{11}, a_{12}, a_{21}, a_{22})$. The order of $GL(2, R)$ is therefore four. If we restrict ourselves to the transformations with $\det(R(a)) = 1$, we obtain a subgroup of $GL(2, R)$, called the *special real linear transformation group* of dimension two, and denoted by $SL(2, R)$.

Example 2: The complex linear transformation group $GL(2, C)$ in two-dimensional space. If the parameters a in (5-25) are allowed to be complex, $R(a)$ form a complex linear transformation group of dimension 2. Let $a_{kl} = b_{kl} + ic_{kl}$, where b_{kl} and c_{kl} are real. Therefore its elements

are characterized by eight real parameters, $a^1 = b_{11}, \ldots, a^8 = c_{22}$, and the order of $GL(2,C)$ is therefore eight.

Example 3: The group SU_2. If the matrices in (5-25) are unitary, that is,

$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} , \tag{5-26a}$$

$$U^\dagger U = 1 , \tag{5-27}$$

then the collection of matrices (5-26a) forms the *unitary group* U_2. If we further restrict the matrices to those satisfying

$$\det(U) = 1 , \tag{5-28}$$

the corresponding group is called the *special unitary group* SU_2.

From (5-26a) and (5-28) we have

$$U^{-1} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} . \tag{5-26b}$$

Moreover from (5-27), (5-26a) and (5-28), we have

$$d = a^*, \quad c = -b^* , \quad |a|^2 + |b|^2 = 1 .$$

Therefore the most general form of the group elements of SU_2 is

$$U = \begin{pmatrix} e^{i\xi}\cos\eta & -e^{i\zeta}\sin\eta \\ e^{i\zeta}\sin\eta & e^{-i\xi}\cos\eta \end{pmatrix} . \tag{5-29}$$

It contains three real parameters ξ, η and ζ. Thus the order of SU_2 is three.

Example 4: The 2-dimensional rotation group R_2. A point $P(x,y)$ in the x-y plane goes to a point $P'(x',y')$ after a rotation through angle φ about the z-axis. From Fig. 5.2, we have

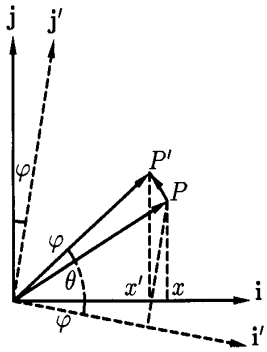


Fig. 5.2. Rotations of points and axes.

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} r\cos(\varphi+\theta) \\ r\sin(\varphi+\theta) \end{pmatrix} = R_z(\varphi)\begin{pmatrix} x \\ y \end{pmatrix} , \tag{5-30a}$$

$$R_z(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} . \tag{5-30b}$$

The matrices $R_z(\varphi)(0 \leq \varphi < 2\pi)$ constitute the 2-dimensional rotation group R_2. $R_z(\varphi)$ in (5-30b) is identical to the rep $D(\varphi)$ of (2-60b) carried by the basis $\varphi_1(x) = x$ and $\varphi_2(x) = y$.

There is only one real parameter, thus $r = 1$. The matrix $R_z(\varphi)$ of (5-30b) is orthogonal, that is,

$$R_z(\varphi)\tilde{R}_z(\varphi) = I\ , \quad \tilde{R}_z^{-1}(\varphi) = R_z(\varphi)\ , \tag{5-31}$$

so R_2 is also called the *special orthogonal group* of dimension 2, or SO_2.

Comparing (5-27) with (5-31) it is seen that if the unitary transformations are restricted to be real, the unitary group degenerates to the orthogonal group. For example, (5-29) goes over to (5-30b) when $\xi = \zeta = 0$, and $\eta = \varphi$.

From Fig. 5.2 it is seen that if the point P is kept fixed and the coordinates axes are rotated through the angle $-\varphi$, then the same relation (5-30) holds between the coordinates x', y' of the same point P in the new axes i' and j', and its old coordinates x, y.

It is easy to see that the hierarchies of the groups so far mentioned are $GL(2,C) \supset GL(2,R) \supset R_2$, and $GL(2,C) \supset U_2 \supset SU_2 \supset R_2$.

Example 5: The 3–dimensional rotation group R_3. In analogy with (5-31), the transformation matrices for rotations through angles α, β, γ about the x, y, z axes, respectively, are

$$R_x(\alpha) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix}\ , \quad R_y(\beta) = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix}\ ,$$
$$R_z(\gamma) = \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}\ . \tag{5-32}$$

Alternatively, we can first rotate the point P through angle γ about the z axis, then rotate through angle β about the y axis, and finally rotate through angle α about the z axis. The set of angles (α, β, γ) are the Euler angles (Rose 1957). As a result of these three rotations, the point P goes to the point P'. The relation between the coordinates of P and P' is

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \mathcal{D}(\alpha\beta\gamma) \begin{pmatrix} x \\ y \\ z \end{pmatrix}\ , \tag{5-33}$$

$$\begin{aligned} \mathcal{D}(\alpha,\beta,\gamma) &= R(\alpha,\beta,\gamma) = R_z(\alpha)R_y(\beta)R_z(\gamma) \\ &= \begin{pmatrix} \cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma, & -\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma, & \cos\alpha\sin\beta \\ \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma, & -\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma, & \sin\alpha\sin\beta \\ -\sin\beta\cos\gamma, & \sin\beta\sin\gamma, & \cos\beta \end{pmatrix}\ . \end{aligned} \tag{5-34}$$

$\mathcal{D}$ is an orthogonal matrix $\mathcal{D}^{-1} = \tilde{\mathcal{D}}$. The Lie group R_3 is also called the special orthogonal group SO_3 of dimension three. In Chapter 6 we discuss this rotation group in more detail.

Let us now consider a new coordinate system $\overline{xyz}$ which is obtained from rotating successively the original coordinate system through angles γ, β and α about the axes z, y, and z, respectively (see the diagram in Bohr 1969, p. 76). From the discussion in Example 4 we know that the relation between the old and new coordinates is given by

$$\begin{pmatrix} \overline{x} \\ \overline{y} \\ \overline{z} \end{pmatrix} = \mathcal{D}^{-1}(\alpha\beta\gamma) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \tilde{\mathcal{D}}(\alpha\beta\gamma) \begin{pmatrix} x \\ y \\ z \end{pmatrix}\ . \tag{5-35}$$

5.3. Lie Algebras

One great contribution of Sophus Lie to the theory of Lie groups was to consider those elements which differ infinitesimally from the identity, and to show that from them one can obtain most of the properties of the Lie group.

We begin with the Taylor expansion of the group elements $R(a)$,

$$R(a) = R(0) + a^\rho X_\rho + \ldots , \tag{5-36}$$

$$X_\rho = \left(\frac{\partial R(a)}{\partial a^\rho} \right)_{a=0} , \tag{5-37}$$

are called *infinitesimal generators* or simply *generators of the Lie group* . For a Lie group of order r, there are r linearly independent generators. To explore the neighborhood of the identity, we only need retain terms linear in a in (5-36), that is,

$$R(a) = 1 + a^\rho X_\rho . \tag{5-38}$$

The inverse element is

$$R^{-1}(a) = 1 - a^\rho X_\rho . \tag{5-39}$$

Suppose that there are two infinitesimal elements and each has only one non-vanishing parameter,

$$R(a) = 1 + \varepsilon X_\rho , \quad R(b) = 1 + \varepsilon X_\sigma . \tag{5-40}$$

According to the definition of the Lie group,

$$\begin{aligned} &R(a)R(b) = R(c) = 1 + C^\tau X_\tau , \\ &R(b)R(a) = R(c') = 1 + C'^\tau X_\tau , \\ &[R(a),\ R(b)] = \varepsilon^2 C^\tau_{\rho\sigma} X_\tau , \end{aligned}$$

$$C^\tau_{\rho\sigma} = (C^\tau - C'^\tau)/\varepsilon^2 . \tag{5-41}$$

On the other hand from (5-40) we have

$$[R(a),\ R(b)] = \varepsilon^2 [X_\rho, X_\sigma] . \tag{5-42}$$

Comparing (5-41) with (5-42), we get an important relation:

$$[X_\rho, X_\sigma] = C^\tau_{\rho\sigma} X_\tau , \tag{5-43}$$

namely, the commutator of two generators is a linear combination of the r generators. The coefficients $C^\tau_{\rho\sigma}$ are called the *structure constants* of the Lie group. They have the following two properties.

1. They are anti-symmetric with respect to the subscripts.

$$C^\tau_{\rho\sigma} = -C^\tau_{\sigma\rho} . \tag{5-44}$$

2. According to the Jacobi identity

$$[[X_\rho, X_\sigma], X_\tau] + [[X_\sigma, X_\tau], X_\rho] + [[X_\tau, X_\rho], X_\sigma] = 0 , \tag{5-45a}$$

we have

$$C^\mu_{\rho\sigma} C^\nu_{\mu\tau} + C^\mu_{\sigma\tau} C^\nu_{\mu\rho} + C^\mu_{\tau\rho} C^\nu_{\mu\sigma} = 0 . \tag{5-45b}$$

The r generators span a real r-dimensional vector space $\mathcal{L}_r$. Any vector in the space can be expressed as $a^\rho X_\rho$. The product of two basis vectors in the space is defined by their commutator (5-43). The set $\{X_\rho\}$ is thus closed under linear combinations and multiplications defined by (5-43), that is, $\{X_\rho\}$ constitutes an algebra and is called the *Lie algebra* corresponding to the given Lie group. If a^ρ are real, it is called a real algebra, otherwise it is a complex Lie algebra.

Results obtained by Lie reduce the searching for irreps of the Lie group with an infinite number of elements, to a search for irreps of the Lie algebra with a finite number of elements. Having found irreps of the Lie algebra, the irreps of the Lie group are also known. Therefore the Lie algebra plays a crucial role in the theory of Lie groups. For a given Lie group, we always first find its corresponding Lie algebra. In physical problems, it often occurs that a certain kind of Lie algebra emerges naturally; nevertheless, the corresponding Lie group does not have a simple physical meaning. In such cases, we only deal with the Lie algebra and do not bother about the related Lie group at all.

In the space $\mathcal{L}_r = \{X_\rho : \rho = 1, 2, \ldots r\}$, any vector can be expressed as

$$X = a^\rho X_\rho \ , \tag{5-46}$$

where a^ρ can be thought of as the coordinates of an abstract vector X. According to (5-2), the basis vectors and the coordinates transform in the following ways:

$$X'_\rho = B_\rho{}^\sigma X_\sigma \ , \quad a'^\rho = A^\rho{}_\sigma a^\sigma , \quad A = \tilde{B}^{-1} \ . \tag{5-47a,b,c}$$

In the new coordinate system with the basis $\{X'_\rho\}$, the structure constants are $C'^{\tau}_{\rho\sigma}$,

$$[X'_\rho, X'_\sigma] = C'^{\tau}_{\rho\sigma} X'_\tau \ . \tag{5-48}$$

From (5-9b), the relation between the new and old structure constants is

$$C'^{\tau}_{\rho\sigma} = B_\rho{}^\mu B_\sigma{}^\nu A^\tau{}_\lambda C^\lambda_{\mu\nu} \ . \tag{5-49}$$

Equation (5-48) shows that the Lie algebra of the same Lie group may take different forms due to the different choices of the group parameters. This point merits special attention when we are dealing with the classification of Lie algebras.

Example 1: The group $GL(2, R)$. Using (5-25) and (5-37) we get the four generators

$$\begin{aligned} X_1 = e_{11} &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} , \quad X_2 = e_{12} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} , \\ X_3 = e_{21} &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} , \quad X_4 = e_{22} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} . \end{aligned} \tag{5-50}$$

It can be shown that those generators obey the following commutation relations:

$$[e_{\alpha\beta}, e_{\gamma\delta}] = \delta_{\beta\gamma} e_{\alpha\delta} - \delta_{\alpha\delta} e_{\gamma\beta} \ . \tag{5-51}$$

Example 2: The group SO_2. From (5-30b) and (5-37) we obtain

$$X_\varphi = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} . \tag{5-52}$$

Example 3: The group SO_3. From (5-32) and (5-37) we have

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} , \quad X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} , \quad X_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} . \tag{5-53a}$$

They obey the commutation relations

$$[X_1, X_2] = X_3 \quad \text{cyclic in 1,2,3} \ . \tag{5-53b}$$

5.4. Finite Transformations

Equation (5-38) is the expression for infinitesimal transformations. Now let us find the expression for finite transformations.

Consider first the single parameter group SO_2. The counterparts of (5-36) and (5-37) are

$$R(\delta\varphi) = 1 + \delta\varphi X_\varphi \ , \quad X_\varphi = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \ . \tag{5-54}$$

Let the infinitesimal angle $\delta\varphi = \varphi/N$, where N is an arbitrarily large number. Therefore

$$R(\delta\varphi) \cong \left(1 + \frac{\varphi}{N} X_\varphi\right) \ .$$

Applying $R(\delta\varphi)$ N times, we obtain the finite rotation

$$\begin{aligned} R(\varphi) &\cong \left(1 + \frac{\varphi}{N} X_\varphi\right)^N = \sum_{n=0}^{N} \binom{N}{n} \left(\frac{\varphi}{N} X_\varphi\right)^n \\ &\underset{N\to\infty}{\to} 1 + \varphi X_\varphi + \frac{\varphi^2}{2!} X_\varphi^2 + \frac{\varphi^3}{3!} X_\varphi^3 + \ldots \\ &= \cos\varphi \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sin\varphi \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} \ . \end{aligned} \tag{5-55}$$

This is the familiar result (5-30b). Equation (5-55) can be written formally as

$$R(\varphi) = e^{\varphi X_\varphi} \ . \tag{5-56}$$

In the above discussion we ignored the unchanged z-component. If the z-component is included, then the generator X_φ in (5-52) goes over to X_3 in (5-53a). Letting $X_3 = -iJ_z$, we get the representative matrix of the operator J_z in the Cartesian coordinate system as shown in (5-58b). The group elements of SO_2 thus take the well-known form

$$R_z(\varphi) = e^{-i\varphi J_z} \ . \tag{5-57}$$

Analogously, we introduce for SO_3

$$X_1 = -iJ_x, \quad X_2 = -iJ_y, \quad X_3 = -iJ_z \ . \tag{5-58a}$$

From (5-53) we have

$$J_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \ , \quad J_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \ , \quad J_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \ . \tag{5-58b}$$

$$[J_x, J_y] = iJ_z, \quad \text{cyclic in } x, y, z \ . \tag{5-59}$$

$J_{x,y,z}$ are the three components of angular momentum . Equation (5-58b) is their matrix representation in the 3-dimensional Cartesian basis.

The rotation operators corresponding to (5-32) are

$$R_x(\alpha) = e^{-i\alpha J_x}, \quad R_y(\beta) = e^{-i\beta J_y}, \quad R_z(\gamma) = e^{-i\gamma J_z} \ . \tag{5-60}$$

The operator for a rotation through angle φ about an axis $\mathbf{n}$ with orientation angle (θ', φ') can be expressed as

$$R_{\mathbf{n}}(\varphi) = e^{-i\varphi \mathbf{n}\cdot\mathbf{J}} = \exp\left[-i\varphi(J_x \sin\theta' \cos\varphi' + J_y \sin\theta' \sin\varphi' + J_z \cos\theta')\right] \ . \tag{5-61}$$

Such a rotation can be written as a product of three rotations

$$R_{\mathbf{n}}(\varphi) = R(\varphi', \theta', 0)R(\varphi, 0, 0)R(0, -\theta', -\varphi') = R(\varphi', \theta', 0)R(\varphi, -\theta', -\varphi') \ , \tag{5-62}$$

namely, first rotate the $\mathbf{n}$–axis onto the z–axis, then rotate through angle φ about the z–axis, and finally bring the z–axis back to the $\mathbf{n}$–axis. Using (5-62) and (5-34) we can get the matrix form of the rotation $R_{\mathbf{n}}(\varphi)$ in the 3–dimensional space x, y and z.

The transition from the infinitesimal transformation (5-54) to the finite transformation can be extended to the more general case

$$R(\delta a) \cong 1 + a^{\rho} X_{\rho}, \quad R(a) = \exp\left(a^{\rho} X_{\rho}\right) . \tag{5-63a, b}$$

It should be mentioned that it is not always possible to write the finite transformation in the form (5-63b). If the transformation can be put in this form, then the group parameters a^{ρ} are said to be *canonical*. For example in (5-61) $a_x = \varphi \sin\theta' \cos\varphi', a_y = \varphi \sin\theta' \sin\varphi', a_z = \varphi \cos\theta'$ are canonical parameters. If we choose the Euler angles α, β and γ as the group parameters of SO_3, from (5-34) and (5-60), we have

$$R(\alpha, \beta, \gamma) = e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z} \ . \tag{5-64}$$

Since J_y and J_z do not commute,

$$R(\alpha, \beta, \gamma) \neq e^{-i(\alpha J_z + \beta J_y + \gamma J_z)} \ .$$

Therefore the Euler angle α, β and γ are not canonical parameters.

5.5. Correspondence between Lie Groups and Lie Algebras

The classifications of Lie groups and Lie algebras are in one-to-one correspondence. This correspondence is based on the two relations (5-65) and (5-66) which follow. Let R_{ρ}, R_{σ} be two infinitesimal elements. Making an expansion of (5-63b) and retaining terms up to ε^2, we obtain

$$R_{\rho} \cong 1 + \varepsilon X_{\rho} + \frac{\varepsilon^2}{2!} X_{\rho}^2, \quad R_{\sigma} \cong 1 + \varepsilon X_{\sigma} + \frac{\varepsilon^2}{2!} X_{\sigma}^2 \ .$$

Therefore

$$[R_{\rho}, R_{\sigma}] = \varepsilon^2 [X_{\rho}, X_{\sigma}] = \varepsilon^2 C_{\rho\sigma}^{\tau} X_{\tau} \ . \tag{5-65}$$

$$R_{\rho} R_{\sigma} R_{\rho}^{-1} R_{\sigma}^{-1} = 1 + \varepsilon^2 [X_{\rho}, X_{\sigma}] = 1 + \varepsilon^2 C_{\rho\sigma}^{\tau} X_{\tau} \ . \tag{5-66}$$

According to the above two relations it is easy to establish the following correspondences:

Lie groups	Lie algebras
1a. Abelian Lie groups	1b. Abelian Lie algebras
$[R_{\rho}, R_{\sigma}] = 0 \ ,$ $\rho, \sigma = 1, 2, \ldots, r \ .$ (5-67a)	$[X_{\rho}, X_{\sigma}] = 0 \ ,$ $\rho, \sigma = 1, 2, \ldots, r \ .$ (5-67b)
2a. Subgroups G_s of a Lie group G. Let $X_i, X_j, \ldots, X_k$ be the generators of G_s. Let $R_i = 1 + \varepsilon X_i, R_j = 1 + \varepsilon X_j$. Therefore	2b. Subalgebras A_s of a Lie algebra A. By (5-68a), $[R_i, R_j]$ is an element of the group algebra of G_s. Using (5-65) we know that $X_i, X_j, \ldots, X_k$ form a subalgebra A_s of A, that is,

$$R_i R_j \in G_s \ . \qquad (5\text{-}68a)$$

3a. Invariant subgroups.
If the elements $R_i, R_j, \ldots, R_k$ belong to an invariant subgroup G_s, one has from (1-28)

$$R_\rho R_i R_\rho^{-1} \in G_s \ , R_i \in G_s \ , \quad \rho = 1, 2, \ldots, r$$

Thus

$$R_\rho R_i R_\rho^{-1} R_i^{-1} \in G_s \ . \qquad (5\text{-}69a)$$

4a. Simple Lie group.
A Lie group which has no invariant subgroups is a simple Lie group.

5a. Semi-simple Lie group.
The Lie group which has no Abelian invariant subgroups is a semi-simple Lie group.

$$[X_i, X_j] \in A_s \ . \qquad (5\text{-}68b)$$

3b. Invariant subalgebras.
From (5-69a) and (5-66) it is known that

$$[X_a, X_\rho] = C_{a\rho}^b X_b \ , \quad a, b = i, j, \ldots, k \ , \ \rho = 1, 2, \ldots, r \ . \qquad (5\text{-}69b)$$

The algebra $X_i, \ldots, X_k$ is called the invariant subalgebra of A.

4b. Simple Lie algebra
A Lie algebra which has no invariant subalgebra is a simple Lie algebra.

5b. Semi-simple Lie algebra.
The Lie algebra which has no Abelian invariant subalgebras is a semi-simple Lie algebra.

6a. **Theorem 5.1:** A semi-simple Lie group is a direct product of a set of simple Lie groups,

$$G = G_1 \times G_2 \times \ldots \times G_n \ , \qquad (5\text{-}70a)$$

where G_i are simple and $[G_i, G_j] = 0$.

6b. **Theorem 5.1′:** A semi-simple Lie algebra is a direct sum of a set of simple Lie algebras,

$$A = A_1 \oplus A_2 \oplus \ldots \oplus A_n \ , \qquad (5\text{-}70b)$$

where A_i are simple, $[A_i, A_j] = 0$ and the intersections between any A_i and A_j are zeroes.

7. A *compact Lie algebra* is one corresponding to a compact Lie group.

It is important to distinguish between the semi-simple and non-semi-simple Lie groups, since Abelian invariant subgroups, though apparently the easiest to deal with, can actually be the most troublesome from the point of view of representations. Fortunately, in most physical applications we deal only with semi-simple Lie groups. Below we mainly concern ourselves with semi-simple Lie groups. (The criteria for semi-simple Lie groups is given in Sec. 5.13.)

In a semi-simple Lie algebra the maximum number of linearly independent generators, denoted $H_1, \ldots, H_l$, which commute with one another, is called the *rank* of the Lie algebra or the rank of the corresponding Lie group, designated by l. (An equivalent definition of rank is given in Sec. 5.18.) . The set of operators $H_1, \ldots H_l$ form a subalgebra, called the *Cartan subalgebra* .

Naturally, any Lie group must be of at least rank 1.

Example 1: For SO_2, there is only one generator J_z. Naturally J_z commutes with itself. Therefore SO_2 is an Abelian group with rank $l = 1$.

Example 2: For SO_3, there are three generators J_x, J_y and J_z. Each of them only commutes with itself. SO_3 is a non-Abelian group of rank 1.

SO_2 and SO_3 are both simple.

5.6 Linear Transformation Groups

In Secs. 5.2 and 5.3, we gave the general definitions of Lie groups and Lie algebras. In Sec. 5.2 we also gave some simple examples. We will now extend these examples to the general linear transformation groups. These groups are the most useful ones in physics. Assume $R(a) = R(a^1, a^2, \ldots, a^r)$ is an n–dimensional linear transformation,

$$x \xrightarrow{R(a)} x' = R(a)x \ , \tag{5-71a}$$

or equivalently

$$x'^{\alpha} = R_{\alpha\beta}(a)x^{\beta}, \quad \alpha = 1, 2, \ldots, n \ . \tag{5-71b}$$

Here x may be real or complex. The set of all $n \times n$ matrices $R(a)$ forms a linear transformation group in n–dimensional space. It can be further classified into the following categories:

1. $GL(n, C) \equiv GL(n)$, the *general complex linear transformation group.* The matrix elements $R_{\alpha\beta}(a)$ are complex numbers. The group contains $2n^2$ real parameters; therefore the order is $r = 2n^2$.

2. $GL(n, R)$, the *general real linear transformation group.* The matrix elements are restricted to real numbers. There are n^2 real parameters. The order is $r = n^2$.

3. $SL(n, C), SL(n, R)$, the *special linear transformation groups.* These two groups are obtained from $GL(n, C)$ and $GL(n, R)$ by requiring that the determinants of the transformations be unity. Their orders are equal to $2n^2 - 2$ and $n^2 - 1$, respectively. Obviously we have

$$GL(n, C) \supset SL(n, C) \supset SL(n, R), \quad GL(n, R) \supset SL(n, R).$$

4. U_n and SU_n, the *unitary group* and *unimodular unitary group* in n dimensions. Restricting matrices $R(a)$ to be unitary, that is,

$$R(a)R^{\dagger}(a) = R^{\dagger}(a)R(a) = I \ , \tag{5-72a}$$

we get the unitary group U_n of order $r = n^2$. The unitary group is compact, since by (5-72a) the matrix elements $|R_{\alpha\beta}(a)| \leq 1$. The condition (5-72a) also stipulates that

$$\det R(a) = \exp(i\varphi) \ . \tag{5-72b}$$

Demanding that the determinants of $R(a)$ equal unity, we obtain the unimodular unitary group SU_n of order $r = n^2 - 1$. The unitarity (5-72a) ensures that the quantity $\sum_{\alpha=1}^{n} |x^{\alpha}|^2$ is an invariant under the unitary transformation,

$$\sum_{\alpha=1}^{n} |x^{\alpha}|^2 = \sum_{\alpha=1}^{n} |x'^{\alpha}|^2 \ . \tag{5-73}$$

The fundamental role of unitary groups in quantum mechanics is easily understood when one realizes that the probabilistic nature of quantum theory requires a preservation of squares of absolute values of various inner product of wave functions.

5. The group $U(n, m)$. All the linear transformations which keep the quantity

$$\sum_{\alpha=1}^{n} |x^{\alpha}|^2 - \sum_{\beta=n+1}^{n+m} |x^{\beta}|^2 \tag{5-74}$$

invariant form the group $U(n, m)$ with order $r = (n + m)^2$. $U(n, m)$ is a noncompact group. Obviously, $U_n = U(n, 0) = U(0, n)$, $GL(n, m) \supset U(n, m)$. Similarly we can define the group $SU(n, m)$, with order $r = (n + m)^2 - 1$.

6. The complex orthogonal group $O(n,C)$. All the complex linear transformations which leave $\sum_{\alpha=1}^{n}(x^{\alpha})^2$ invariant form the complex orthogonal group. From

$$\sum_{\alpha=1}^{n}(x'^{\alpha})^2 = \sum_{\alpha\beta\beta'} R_{\alpha\beta}R_{\alpha\beta'}x^{\beta}x^{\beta'} = \sum_{\beta=1}^{n}(x^{\beta})^2 , \tag{5-75}$$

we have

$$\sum_{\alpha} R_{\alpha\beta}R_{\alpha\beta'} = \delta_{\beta\beta'} . \tag{5-76a}$$

Thus $R(a)$ are orthogonal matrices,

$$\tilde{R}(a)R(a) = 1 . \tag{5-76b}$$

$O(n,C)$ has $n(n-1)/2$ complex parameters (see Sec. 5.8), therefore it is of order $r = n(n-1)$. From (5-76b) we have

$$\det\big(\tilde{R}(a)\big)\det\big(R(a)\big) = 1 , \quad \det\big(R(a)\big) = \pm 1 . \tag{5-76c}$$

The transformation matrices of $O(n,C)$ can be divided into two sets, one is associated with $\det\big(R(a)\big) = +1$, and the other with $\det\big(R(a)\big) = -1$. The set with determinant $+1$ forms a subgroup respreseting *proper rotations*, the *unimodular complex orthogonal group* $SO(n,C)$. We can decompose the group $O(n,C)$ into cosets with respect to the subgroup $SO(n,C)$, that is,

$$O(n,C) = SO(n,C) \oplus SO(n,C) \times I , \tag{5-77}$$

where I is the space inversion operator.

The quotient group $O(n,C)/SO(n,C)$ is a group of order 2. The set with determinant -1 represents rotation-reflections. Any element of $SO(n,C)$ can be reached from the identity via continuous paths in parameter space, while the elements with $\det\big(R(a)\big) = -1$ cannot. In other words, the group $O(n,C)$ consists of two disconnected parts and we cannot go from one part to the other continuously.

7. The real orthogonal group O_n. Restricting the matrices of $O(n,C)$ to be real leads to the real orthogonal group, denoted by O_n or $O(n)$, which is of order $r = \frac{1}{2}n(n-1)$. By further requiring $\det\big(R(a)\big) = 1$, we get the unimodular orthogonal group SO_n. It is still of order $\frac{1}{2}n(n-1)$. Similarly, the group O_n also consists of two disconnected parts. Obviously we have

$$O(n,C) \supset SO(n,C) \supset SO_n , \quad O_n \supset SO_n .$$

8. The group $O(n,m)$.

All the real linear transformation which leave the quantity

$$\sum_{\alpha=1}^{n}(x^{\alpha})^2 - \sum_{\beta=n+1}^{n+m}(x^{\beta})^2 \tag{5-78}$$

invariant form the group $O(n,m)$ with order $r = \frac{1}{2}[n(n-1) + m(m-1)] + nm$. $O(n,m)$ is a noncompact group. The Lorentz group $O(3,1)$ is a special case of $O(n,m)$.

Obviously, we have $O_n = O(n,0) = O(0,n)$.

9. *Complex symplectic, real symplectic* and *unitary symplectic groups* $Sp(2n,C)$, $Sp(2n,R)$, and Sp_{2n}.

Suppose $\mathbf{x} = (x^1,\ldots,x^n;x^{-1},\ldots,x^{-n})$ and $\mathbf{y} = (y^1,\ldots,y^n;y^{-1},\ldots y^{-n})$ are two column vectors with dimension $2n$ and $R(a)$ are $2n \times 2n$ matrices, which transform $\mathbf{x}$ and $\mathbf{y}$ into $\mathbf{x}'$ and $\mathbf{y}'$:

$$\mathbf{x}' = R(a)\mathbf{x}, \quad \mathbf{y}' = R(a)\mathbf{y} . \tag{5-79a}$$

The symplectic group is the set of all $2n \times 2n$ linear transformations $R(a)$ which leave the skew-symmetric bilinear form

$$\sum_{\alpha=1}^{n}(x^{\alpha}y^{-\alpha} - x^{-\alpha}y^{\alpha}) \tag{5-79b}$$

invariant. If the $2n \times 2n$ matrices $R(a)$ are complex (real), it is called the *complex* (real) *symplectic group* of order $2n(2n+1)\big(n(2n+1)\big)$. If the complex matrices $R(a)$ are unitary, the group is called the *unitary symplectic group* Sp_{2n} . We have

$$GL(2n,C) \supset Sp(2n,C) \supset Sp(2n,R), \quad Sp(2n,C) \supset Sp_{2n}, \quad SU_{2n} \supset Sp_{2n} .$$

The groups $Sp(2n,C)$ and $Sp(2n,R)$ are noncompact, while Sp_{2n} is compact.

5.7. Infinitesimal Operators for Linear Transformation Groups

Consider subjecting $x^1, x^2, \ldots, x^n$ to an infinitesimal transformation

$$x' = R(a)x, \quad R(a) = 1 + \mathcal{A}(a) , \tag{5-80a}$$

$$\mathcal{A}(a) = \sum_{\alpha\beta} a_{\alpha\beta}e_{\alpha\beta} , \tag{5-81}$$

where $a_{\alpha\beta}$ are infinitesimal quantities and $e_{\alpha\beta}$ are the $n \times n$ matrices defined in (2-4). The $e_{\alpha\beta}$ obey the commutator (5-51) and the following relation

$$e_{\alpha\beta}e_{\gamma\delta} = \delta_{\beta\gamma}e_{\alpha\delta} . \tag{5-82}$$

Equation (5-80a) can also be rewritten as

$$x'^{\alpha} = x^{\alpha} + a^{\alpha}{}_{\beta}x^{\beta} . \tag{5-80b}$$

Under the transformation (5-80b), an arbitrary function $\psi(x)$ goes over to

$$\psi'(x) = \psi(x') = \psi(x^{\alpha} + a^{\alpha}{}_{\beta}x^{\beta}) = \psi(x) + a^{\alpha}{}_{\beta}\, x^{\beta}\frac{\partial}{\partial x^{\alpha}}\psi(x) . \tag{5-83}$$

Defining the infinitesimal operators

$$E_{\beta\alpha} = x^{\beta}\frac{\partial}{\partial x^{\alpha}} , \tag{5-84}$$

Eq. (5-83) reads

$$\psi'(x) = (1 + a^{\alpha}{}_{\beta}E_{\beta\alpha})\psi(x) = (1 + a^{\rho}X_{\rho})\psi(x) , \tag{5-85}$$

and (5-80b) can be expressed as

$$x'^{\alpha} = \Big(1 + \sum_{\beta} a^{\alpha}{}_{\beta}E_{\beta\alpha}\Big)x^{\alpha} . \tag{5-80c}$$

From this we obtain a simple method for finding the infinitesimal operators of the linear transformation group:

1. First find the infinitesimal matrix $\mathcal{A}$ in the infinitesimal transformations (5-80a), that is,

$$\mathcal{A} = \sum_{\alpha\beta} a^{\alpha}{}_{\beta}e_{\alpha\beta} . \tag{5-86a}$$

Notice that not all the parameters $a_{\alpha\beta}$ are independent, except for the group $GL(n,R)$ or $GL(n,C)$.

2. Replacing $e_{\alpha\beta}$ by the differential operator $E_{\beta\alpha}$ of (5-84); Eq. (5-86a) becomes

$$\sum_{\alpha\beta} a^{\alpha}_{\ \beta} E_{\beta\alpha} \ . \tag{5-86b}$$

3. Expressing the parameters $a_{\alpha\beta}$ in terms of the independent parameters $a^1, a^2, \ldots, a^r$ and setting in turn

$$a^{\rho} = 1, \quad a^{\sigma} = 0, \quad \text{for } \sigma \neq \rho, \quad \rho = 1, 2, \ldots, r,$$

we can obtain the r infinitesimal operators X_{ρ}.

Example. Find the infinitesimal operators of SO_3. According to (5-76), we have

$$\tilde{R}(a)R(a) = [1 + \tilde{\mathcal{A}}(a)][1 + \mathcal{A}(a)] \cong 1 + \tilde{\mathcal{A}}(a) + \mathcal{A}(a) = 1 \ .$$

Therefore

$$\tilde{\mathcal{A}}(a) + \mathcal{A}(a) = 0 \ . \tag{5-87}$$

Thus $\mathcal{A}(a)$ is an anti-symmetric matrix, and must have the form:

$$\begin{aligned} \mathcal{A}(a) &= \begin{pmatrix} 0 & a^3 & -a^2 \\ -a^3 & 0 & a^1 \\ a^2 & -a^1 & 0 \end{pmatrix} \\ &= a^1(e_{23} - e_{32}) + a^2(e_{31} - e_{13}) + a^3(e_{12} - e_{21}) \\ &\to a^1(E_{32} - E_{23}) + a^2(E_{13} - E_{31}) + a^3(E_{21} - E_{12}) \ . \end{aligned} \tag{5-88}$$

Letting $(a^1, a^2, a^3) = (1, 0, 0), (0, 1, 0)$ and $(0, 0, 1)$, we obtain the three infinitesimal operators of SO_3.

$$\begin{aligned} X_1 &= E_{32} - E_{23} = z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z} \ , \\ X_2 &= E_{13} - E_{31} = x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x} \ , \\ X_3 &= E_{21} - E_{12} = y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} \ . \end{aligned} \tag{5-89}$$

If we set $X_k = -iJ_k$, we get the differential form of the angular momentum operators:

$$J_x = i\left(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right) \ , \quad \text{cyclic in } x, y, z \ . \tag{5-90}$$

From the above example it is seen that the infinitesimal operators can be written down immediately once the infinitesimal matrix $\mathcal{A}$ was known.

Comparing (5-58b) with (5-90), we see that the former represents the angular momentum operators in the Cartesian basis, while the latter describe the angular momentum operators acting on wave function $\psi(x, y, z)$. It is easy to show that the differential operators $E_{\alpha\beta}$ in (5-84) and the matrices $e_{\alpha\beta}$ in (2-4) have the same commutators:

$$[E_{\alpha\beta}, E_{\gamma\delta}] = \delta_{\beta\gamma}E_{\alpha\delta} - \delta_{\alpha\delta}E_{\gamma\beta} \ . \tag{5-91}$$

If the n single particle states $\varphi_1, \varphi_2, \ldots, \varphi_n$ are chosen as the basis in an n-dimensional space, the linear transformation (5-80c) becomes

$$\varphi'_{\alpha}(i) = \varphi_{\alpha}(i) + \sum_{\beta=1}^{n} a_{\alpha\beta}\varphi_{\beta}(i) \ , \tag{5-92a}$$

where i is the particle index.

We now introduce the creation and annihilation operators $c^\dagger_\alpha(i)$ and $c_\beta(i)$ for the particle i,

$$c^\dagger_\alpha(i)|0\rangle = \varphi^i_\alpha \qquad c_\alpha(i)|0\rangle = 0 \ . \tag{5-93a}$$

Those operators obey the commutators

$$[c^\dagger_\alpha(i), c^\dagger_\beta(i)] = 0, \qquad [c_\alpha(i), c^\dagger_\beta(j)] = \delta_{ij}\delta_{\alpha\beta} \ . \tag{5-93b}$$

Equation (5-92a) can be rewritten as

$$\varphi'_\alpha(i) = \Big(1 + \sum_\beta a_{\alpha\beta} c^\dagger_\beta(i) c_\alpha(i)\Big)\varphi_a(i) \ . \tag{5-92b}$$

Comparing (5-92b) with (5-80c), we see that acting on the single particle states, the infinitesimal operators $E_{\alpha\beta}$ take the form,

$$e^{(i)}_{\alpha\beta} = c^\dagger_\alpha(i) c_\beta(i) \ . \tag{5-94a}$$

The operators $e^{(i)}_{\alpha\beta}$ are the infinitesimal operators acting on the ith particle state,

$$e^{(i)}_{\alpha\beta}\varphi^{(j)}_\gamma = \delta_{ij}\delta_{\beta\gamma}\varphi^{(i)}_\alpha \ . \tag{5-94b}$$

and they obey the relations

$$e^{(i)}_{\alpha\beta} e^{(i)}_{\gamma\delta} = \delta_{\beta\gamma} e^{(i)}_{\alpha\delta} \ , \tag{5-94c}$$

$$[e^{(i)}_{\alpha\beta}, e^{(j)}_{\gamma\delta}] = \delta_{ij}(\delta_{\beta\gamma} e^{(i)}_{\alpha\delta} - \delta_{\alpha\delta} e^{(i)}_{\gamma\beta}) \ . \tag{5-94d}$$

The elements of $GL(n, C)$ for finite parameters $a_{\alpha\beta}$ are

$$R^{(i)}(a) = \exp\Big[-i \sum_{\alpha\beta} a_{\alpha\beta} e^{(i)}_{\alpha\beta}\Big] \ , \tag{5-95}$$

The action of the group element $R(a)$ on the n–particle product states is defined as inducing a linear transformation on all the single particle states:

$$R(a)\big(\varphi_{m_1}(1)\ldots\varphi_{m_n}(n)\big) = \big(R^{(1)}(a)\varphi^{m_1}\big)\ldots\big(R^{(n)}(a)\varphi_{m_n}(n)\big) \ . \tag{5-96a}$$

The elements of $GL(n, C)$ acting on many–particle states are

$$R(a) = \prod_{i=1}^{n} R^{(i)}(a) = \exp\Big(-i \sum_{\alpha\beta} a_{\alpha\beta}\mathcal{E}_{\alpha\beta}\Big) \ , \tag{5-96b}$$

$$\mathcal{E}_{\alpha\beta} = \sum_{i=1}^{n} e^{(i)}_{\alpha\beta} = \sum_{i=1}^{n} c^\dagger_\alpha(i) c_\beta(i) \ . \tag{5-96c}$$

The $\mathcal{E}_{\alpha\beta}$ are the generators of the unitary group acting on many–particle states. Using (5-94c) it is easy to show that

$$[\mathcal{E}_{\alpha\beta}, \mathcal{E}_{\gamma\delta}] = \delta_{\beta\gamma}\mathcal{E}_{\alpha\delta} - \delta_{\alpha\delta}\mathcal{E}_{\gamma\beta} \ . \tag{5-97}$$

In other words, the operators $\mathcal{E}_{\alpha\beta}$ obey the same commutator as the operators $e_{\alpha\beta}$, however, (5-94c) is no longer true. Now $\mathcal{E}_{\alpha\beta}\mathcal{E}_{\gamma\delta} \neq \delta_{\beta\gamma}\mathcal{E}_{\alpha\delta}$, due to the occurrence of cross terms like $e^{(a_i)}_{\alpha\beta} e^{(a_j)}_{\gamma\delta}$.

In the future, we no longer distinguish between the generator $e_{\alpha\beta}$ and the infinitesimal operator $E_{\alpha\beta}$. Depending on the case under study $e_{\alpha\beta}$ may take the following different forms:

$$x^{\alpha}\frac{\partial}{\partial x^{\beta}}, \quad \sum_i c_{\alpha}^{\dagger}(i)c_{\beta}(i)\ , \quad c_{\alpha}^{\dagger}c_{\beta}\ , \quad \begin{pmatrix} & \beta\text{–th column} & \\ & \vdots & \\ \ldots & 1 & \ldots \\ & \vdots & \end{pmatrix} \alpha\text{–th row}\ . \tag{5-98}$$

The form $e_{\alpha\beta} = c_{\alpha}^{\dagger}c_{\beta}$ is the most convenient one for calculating commutators.

5.8. The Metric Tensor in n–Dimensional Space and Infinitesimal Operators

In Sec. 5.7 it was demonstrated that once the infinitesimal matrix $\mathcal{A}(a)$ is known, the infinitesimal operators can be found immediately. We are now going to discuss the problem of how to construct the infinitesimal matrix from the metric tensor $g_{\alpha\beta}$ in n–dimensional space.

Given a set of basis vectors $\{\mathbf{u}_{\alpha}\}$ and a *metric tensor* $g_{\alpha\beta}$ in an n–dimensional space, an invariant is specified, either in the form of

$$x^{\alpha *}g_{\alpha\beta}x^{\beta} = x'^{\alpha *}g_{\alpha\beta}x'^{\beta} \tag{5-99a}$$

for the sesquilinear metric, or

$$x^{\alpha}g_{\alpha\beta}x^{\beta} = x'^{\alpha}g_{\alpha\beta}x'^{\beta} \tag{5-99b}$$

for the bilinear metric. From Sec. 5.6 we know that all the transformations $x' = R(a)x$ which leave a quantity invariant form a Lie group. Therefore a metric tensor corresponds to a Lie group. For the sesquilinear metric, from (5-99a) we have

$$x^{\alpha *}g_{\alpha\delta}x^{\delta} = x'^{\beta *}g_{\beta\gamma}x'^{\gamma} = R_{\beta\alpha}^{*}(a)x^{\alpha *}g_{\beta\gamma}R_{\gamma\delta}(a)x^{\delta}\ . \tag{5-100}$$

Therefore

$$g_{\alpha\delta} = R_{\beta\alpha}^{*}(a)g_{\beta\gamma}R_{\gamma\delta}(a)\ . \tag{5-101}$$

That is,

$$g = R^{\dagger}(a)gR(a)\ . \tag{5-102}$$

Substituting

$$R(a) = 1 + iB(a) \tag{5-102'}$$

into (5-102), where $B(a)$ is an infinitesimal matrix, and neglecting the second order term, we have

$$B^{\dagger}(a)g = g\,B(a)\ . \tag{5-103}$$

Analogously, for the bilinear metric, from (5-99b) we have

$$g = \tilde{R}(a)\,g\,R(a)\ . \tag{5-104}$$

Letting $R = 1 + \mathcal{A}(a)$ we have

$$\tilde{\mathcal{A}}(a)g = -g\mathcal{A}(a)\ , \text{ or } \mathcal{A}(a) = -g^{-1}\tilde{\mathcal{A}(a)}g\ , \tag{5-105}$$

which may be written as

$$a_{\alpha\beta}g_{\alpha\gamma} = -g_{\beta\alpha}a_{\alpha\gamma}\ . \tag{5-106}$$

Equations (5-103) and (5-105) are our starting points for determining the infinitesimal matrices from the given metric tensor.

5.8.1. Unitary groups

Comparing (5-99a) with (5-73) it is seen that the sesquilinear symmetric metric

$$g_{\alpha\beta} = \delta_{\alpha\beta} \tag{5-107}$$

corresponds to the unitary group. According to (5-103) and (5-107), the infinitesimal matrix $B(a)$ must be hermitian, that is,

$$B^{\dagger}(a) = B(a) \ . \tag{5-108}$$

As an example, for the group U_3, $B(a)$ takes the form

$$B(a) = \begin{pmatrix} c_1 & a_1 - ib_1 & a_2 - ib_2 \\ a_1 + ib_1 & c_2 & a_3 - ib_3 \\ a_2 + ib_2 & a_3 + ib_3 & c_3 \end{pmatrix} \ . \tag{5-109}$$

By setting one of the nine parameters $a_1, \ldots, c_3$ equal to 1 and all the others equal to zero successively, we obtain the following nine infinitesimal operators.

$$\begin{aligned} X_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad X_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \\ X_4 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad X_5 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad X_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \\ X_7' &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad X_8' = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad X_9' = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} . \end{aligned} \tag{5-110}$$

For unitary groups we often choose real infinitesimal operators $e_{\alpha\beta}$ [see (5-81)],

$$R(a) = 1 - i \sum_{\alpha\beta} a_{\alpha\beta} e_{\alpha\beta} \ . \tag{5-111}$$

Now the parameters $a_{\alpha\beta}$ become complex and obey $a^*_{\alpha\beta} = a_{\beta\alpha}$.

It is readily seen that the unit matrix $I = \sum_{\alpha=1}^{n} e_{\alpha\alpha}$ is an invariant subalgebra of U_n; therefore U_n is not semi-simple.

Since $x_\alpha x^\alpha = \sum_\alpha (x^\alpha)^* x^\alpha$ is an invariant of U_n, the covariant variables x_α are the complex conjugate of the contravariant variables x^α,

$$x_\alpha = x^{\alpha *} \ . \tag{5-112}$$

We can also introduce the mixed-type metric tensor g^β_α through the invariant

$$x^\alpha x_\alpha = x^\alpha g^\beta_\alpha x_\beta \ . \tag{5-113}$$

Therefore

$$g^\beta_\alpha = \delta_{\alpha\beta} \ . \tag{5-114}$$

It is easy to show that g^β_α is an invariant, that is,

$$g'^\beta_\alpha = R_{\beta\delta} R^*_{\alpha\gamma} g^\delta_\gamma = R_{\beta\delta} R^*_{\alpha\delta} = \delta_{\alpha\beta} \ . \tag{5-115}$$

A mixed tensor can be constructed out of p contravariant vectors and q covariant vectors:

$$T^{\alpha\beta\ldots\gamma}_{ij\ldots k} = x^\alpha y^\beta \ldots z^\gamma u_i v_j \ldots w_k \ . \tag{5-116}$$

An anti–symmetric contravariant tensor is defined by

$$\varepsilon^{i_1 i_2 \ldots i_n} = \begin{cases} 1, & \text{if } p = \begin{pmatrix} 1 & 2 \ldots n \\ i_1 & i_2 \ldots i_n \end{pmatrix} \text{ is } \begin{matrix} \text{even}, \\ \text{odd}, \end{matrix} \\ -1 \\ 0 \quad \text{if any two indices are equal} \end{cases} \tag{5-117}$$

An anti–symmetric covariant tensor $\varepsilon_{i_1, i_2 \ldots i_n}$ can be defined in the same way. Under the U_n transformation

$$\begin{aligned} & \varepsilon^{i_1 i_2 \ldots i_n} \to \varepsilon^{'i_1 i_2 \ldots i_n} \\ &= \sum_{j_1 \ldots j_n} R_{i_1 j_1}(a) R_{i_2 j_2}(a) \ldots R_{i_n j_n}(a) \varepsilon^{j_1 j_2 \ldots j_n} \\ &= \det\left(R(a)\right) \varepsilon^{i_1 i_2 \ldots i_n} . \end{aligned} \tag{5-118}$$

Thus the anti–symmetric contravariant tensor $\varepsilon^{i_1, i_2 \ldots i_n}$ is at the same time an invariant of SU_n. The same is true for the anti–symmetric covariant tensor $\varepsilon_{i_1 i_2 \ldots i_n}$.

5.8.2. Infinitesimal operators of SU_n

The group SU_n demands that $\det\left(R(a)\right) = 1$. The SU_n is simple and belongs to the classical group A_{n-1} with rank $l = n - 1$.

For infinitesimal elements we have

$$\det\left(R(a)\right) = \det\left(1 + iB\right) = 1 + i \sum_{\alpha} B_{\alpha\alpha} + \ldots = 1 . \tag{5-119}$$

Therefore

$$\operatorname{Trace} B = 0 . \tag{5-120}$$

Thus for SU_2, B takes the form

$$B = \begin{pmatrix} c & a - ib \\ a + ib & -c \end{pmatrix} . \tag{5-121}$$

Letting $(a, b, c) = (1, 0, 0), (0, 1, 0), (0, 0, 1)$, we get three infinitesimal operators

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{5-122}$$

These are the Pauli matrices.

Of the nine operators $X_1, \ldots, X_9$ in (5-110), the first six are already traceless, while X_7', X_8' and X_9' can be combined into a unit matrix and two traceless matrices, which can be chosen as

$$X_7 = \sqrt{\frac{1}{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} , \quad X_8 = \sqrt{\frac{1}{6}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} . \tag{5-123}$$

The choice of traceless matrices is not unique.

For the group SU_n, the infinitesimal operators can also be chosen to be real. The non–diagonal operators are $e_{\alpha\beta}$, while the diagonal ones can be chosen in many ways. The most usual choices are as follows:

1.Choose the n commuting operators as

$$h_i = e_{ii} - \frac{1}{n} \sum_{j=1}^{n} e_{jj} , \quad i = 1, 2, \ldots, n . \tag{5-124}$$

Among the n operators, only $(n-1)$ h_i's are independent due to

$$\sum_{i=1}^{n} h_i = 0 \,. \tag{5-125}$$

2. Another choice is cited below but the discussion for the motivation of this choice is postponed to Sec. 5.9 (see Eq. (5-157b)). Let $n = 2a+1$, The $n-1$ commuting operators as

$$h_r = \sum_{\alpha=-a}^{a} C^{r\ 0}_{a\alpha,a-\alpha}(-1)^{(a-\alpha)} e_{\alpha\alpha},\ r = 1,2,\ldots,n-1 \,, \tag{5-126}$$

where $C^{r\ 0}_{a\alpha,a-\alpha}$ is the SO_3 Clebsch-Gordan coefficients. For example, the operators h_1 and h_2 for SU_3 are precisely the operators X_7 and X_8 in (5-123), and for SU_4 we have

$$h_1 = \frac{1}{\sqrt{20}}\{3,1,-1,-3\}_{\text{diag}},\quad h_2 = \frac{1}{2}\{1,-1,-1,1\}_{\text{diag}},\quad h_3 = \frac{1}{\sqrt{20}}\{1,-3,3,-1\}_{\text{diag}}, \tag{5-127}$$

where $\{a,b,c,d\}_{\text{diag}}$ stands for a diagonal matrix with row (column) indexed as $\alpha = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$.

5.8.3. The group $U(n,m)$

From (5-74) and (5-99a) one sees that the matrix tensor is

$$g_{\alpha\beta} = \delta_\alpha \delta_{\alpha\beta},\quad \delta_\alpha = \begin{cases} 1, & \alpha = 1,2,\ldots,n \\ -1, & \alpha = n+1, n+2,\ldots,\ldots,n+m \end{cases} . \tag{5-128}$$

According to (5-103) and (5-128), the infinitesimal elements of the group $U(n,m)$ must take the form

$$R(a) = 1 + i\left(\begin{array}{c|c} B_n & B_{nm} \\ \hline B_{mn} & B_m \end{array}\right) , \tag{5-129}$$

$$B_n = B_n^\dagger ,\quad B_m = B_m^\dagger ,\quad B_{nm} = -B_{mn}^\dagger , \tag{5-130}$$

where B_n, B_m and B_{nm} are $n\times n, m\times m$ and $n\times m$ matrices, respectively. From (5-129), it is easy to write down the infinitesimal operators of $U(n,m)$. $U(n,m)$ is of order $r = n^2 + m^2 + 2nm = (n+m)^2$. For the group $SU(n,m)$, we have the further restriction

$$\text{Tr } B_n + \text{Tr } B_m = 0 \,, \tag{5-131}$$

so that

$$r = (n+m)^2 - 1 \,. \tag{5-132}$$

5.8.4. The orthogonal group O_n

1. Cartesian basis

Comparing (5-75) with (5-99b), we know that the bilinear symmetric metric

$$g_{\alpha\beta} = \delta_{\alpha\beta} \tag{5-133}$$

corresponds to the orthogonal group. Therefore the covariant and contravariant vectors coincide. From (5-105) and (5-133) we know that $\mathcal{A}$ is an anti-symmetric matrix

$$\tilde{\mathcal{A}} = -\mathcal{A} \tag{5-134}$$

with $r = \frac{1}{2}n(n-1)$ real parameters. Consequently

$$\mathcal{A} = \sum_{\alpha>\beta=1}^{n} a_{\beta\alpha}(e_{\beta\alpha} - e_{\alpha\beta}) \to \sum_{\alpha>\beta=1} a_{\beta\alpha}(E_{\alpha\beta} - E_{\beta\alpha}) \,. \tag{5-135}$$

The infinitesimal operators of O_n follow from (5-135) and (5-84):

$$L_{\alpha\beta} = -L_{\beta\alpha} = x_a \frac{\partial}{\partial x_\beta} - x_\beta \frac{\partial}{\partial x_a} = c_\alpha^\dagger c_\beta - c_\beta^\dagger c_\alpha \ . \tag{5-136}$$

Using (5-91) we obtain the commutator relation

$$[L_{\alpha\beta}, L_{\gamma\delta}] = \delta_{\beta\gamma} L_{\alpha\delta} + \delta_{\alpha\delta} L_{\beta\gamma} + \delta_{\beta\delta} L_{\gamma\alpha} + \delta_{\alpha\gamma} L_{\delta\beta} \ . \tag{5-137}$$

Equation (5-137) is the extension of (5-89) of O_3.

2. Spherical basis. See Eq. (5-168).

The group O_{2l+1} belongs to the classical group B_l of rank l and the group O_{2l} belongs to the classical group D_l of rank l (see Sec. 5.20).

5.8.5 The real orthogonal group $O(n,m)$

The metric tensor is determined by the invariant (5-78),

$$g_{\alpha\beta} = \delta_\alpha \delta_{\alpha\beta} \ , \quad \delta_\alpha = \begin{cases} 1, & \alpha = 1,2,\ldots,n \\ -1, & \alpha = n+1,\ldots,n+m \ . \end{cases} \tag{5-138}$$

From (5-106) and (5-138) we have

$$\delta_\alpha a_{\alpha\beta} = -\delta_\beta a_{\beta\alpha} \ . \tag{5-139}$$

Therefore

$$\mathcal{A}(a) = \begin{pmatrix} \mathcal{A}_n & \mathcal{A}_{nm} \\ \tilde{\mathcal{A}}_{nm} & \mathcal{A}_m \end{pmatrix} \ , \quad \mathcal{A}_n = -\tilde{\mathcal{A}}_n, \quad \mathcal{A}_m = -\tilde{\mathcal{A}}_m \ . \tag{5-140}$$

The anti-symmetric matrices $\mathcal{A}_n$ and $\mathcal{A}_m$ have $\frac{1}{2}n(n-1)$ and $\frac{1}{2}m(m-1)$ parameters, respectively and $\mathcal{A}_{nm}$ has nm parameters. Therefore the order of the group $O(n,m)$ is

$$r = \frac{1}{2}[n(n-1) + m(m-1)] + mn = \frac{1}{2}(m+n)(m+n-1) \ . \tag{5-141}$$

With the help of (5-139), we can immediately write down the infinitesimal operators of $O(n,m)$, that is,

$$L_{\alpha\beta} = \delta_\alpha x^\alpha \frac{\partial}{\partial x^\beta} - \delta_\beta x^\beta \frac{\partial}{\partial x^\alpha} = \delta_\alpha c_\alpha^\dagger c_\beta - \delta_\beta c_\beta^\dagger c_\alpha \ . \tag{5-142}$$

Example 3: The Lorentz group $O(3,1)$. Here $n = 3, m = 1$ and $r = 6$. The six infinitesimal operators are

$$\begin{aligned} L_{ij} &= x^i \frac{\partial}{\partial x^j} - x^j \frac{\partial}{\partial x^i}, \quad i,j = 1,2,3 \ . \\ L_{i4} &= x^i \frac{\partial}{\partial x^4} + x^4 \frac{\partial}{\partial x^i}, \quad i = 1,2,3 \ . \end{aligned} \tag{5-143}$$

The complex orthogonal group $O(n,m,C)$ can be handled in the same way. The infinitesimal matrices $\mathcal{A}(a)$ still have the form (5-140). However $\mathcal{A}(a)$ is now complex and the number of parameters is doubled.

5.8.6. Symplectic groups

1. The real symplectic group $Sp(2n,R)$

From the invariant (5-79) we obtain the metric tensor

$$g_{\alpha\beta} = \varepsilon_{\alpha\beta} = -\varepsilon_{\beta\alpha} = \delta_a \delta(\alpha+\beta) \ , \quad \delta(\alpha+\beta) = \delta_{\alpha-\beta} \ ,$$

$$\varepsilon_{\alpha\beta} = \begin{cases} \delta_\alpha, & \alpha = -\beta \ , \\ 0, & \alpha \neq -\beta \ , \end{cases} \quad \delta_\alpha = \text{sign}(\alpha) \ . \tag{5-144}$$

Therefore the bilinear anti-symmetric metric corresponds to the symplectic group. The infinitesimal matrix satisfies the conditions

$$\delta_\alpha a_{\alpha\beta} = -\delta_\beta a_{-\beta-\alpha} \ . \tag{5-145}$$

Therefore $\mathcal{A}(a)$ must be of the form

$$\mathcal{A} = \begin{array}{c} \\ \\ \end{array} \begin{array}{c} 1 \ldots n, \quad -1 \ldots -n \\ \left(\begin{array}{cc} \mathcal{A}_1 & \mathcal{A}_2 \\ \mathcal{A}_3 & -\tilde{\mathcal{A}}_1 \end{array} \right) \end{array} , \quad \mathcal{A}_2 = \tilde{\mathcal{A}}_2, \ \mathcal{A}_3 = \tilde{\mathcal{A}}_3 \ . \tag{5-146}$$

Notice that $\mathcal{A}(a)$ is traceless, therefore the symplectic matrices are unimodular. The infinitesimal operators are

$$\begin{aligned} L_{\alpha\beta} &= \delta_\alpha c_\alpha^\dagger c_\beta - \delta_\beta c_{-\beta}^\dagger c_{-\alpha} \ , \\ L_{\alpha\beta} &= L_{-\beta-\alpha}, \quad \alpha, \beta = \pm 1, \ldots, \pm n \ . \end{aligned} \tag{5-147}$$

The matrix $\mathcal{A}_1$ has n^2 parameters and the symmetric matrices $\mathcal{A}_2$ and $\mathcal{A}_3$ each has $\frac{1}{2}n(n+1)$ parameters. The group $Sp(2n, R)$ is of order

$$r = n^2 + n(n+1) = n(2n+1) \ . \tag{5-148}$$

The generators obey the commutators

$$\begin{aligned} [L_{\alpha\beta}, L_{\gamma\delta}] &= \delta_{\beta\gamma}\delta_\beta L_{\alpha\delta} - \delta_{\alpha\delta}\delta_\alpha L_{\gamma\beta} + \delta_{\beta\overline{\delta}}\delta_\beta L_{\alpha\overline{\gamma}} - \delta_{\alpha\overline{\gamma}}\delta_\alpha L_{\overline{\beta}\gamma} \ , \\ [L_{\alpha\beta}, L_{\beta\gamma}] &= \delta_\beta L_{\alpha\gamma} - \delta_{\alpha\gamma}\delta_\alpha L_{\beta\beta} \ , \end{aligned} \tag{5-149}$$

where $\overline{\beta} = -\beta$ and so on, and

$$[L_{\alpha\beta}, L_{\gamma\delta}] = 0,$$

for different $|\alpha|, |\beta|, |\gamma|, |\delta|$.

Among the r infinitesimal operators of (5-147), the following n operators H_i commute with one another:

$$H_i = L_{ii}, \quad i = 1, 2, \ldots, n \ . \tag{5-150}$$

Therefore the rank of $Sp(2n, R)$ is n.

Example 4: $Sp(4, R)$ has ten parameters. From (5-146) we have

$$\mathcal{A} = \begin{array}{c} \\ 1 \\ 2 \\ -1 \\ -2 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & -1 & -2 \end{array} \\ \begin{pmatrix} e_1 & \alpha & \gamma & \beta \\ \overline{\alpha} & e_2 & \beta & \delta \\ \overline{\gamma} & \overline{\beta} & -e_1 & \overline{\alpha} \\ \overline{\beta} & \overline{\delta} & -\alpha & -e_2 \end{pmatrix} \end{array} . \tag{5-151}$$

The ten infinitesimal operators of $Sp(4, R)$ are

$$H_1 = L_{11}, \quad H_2 = L_{22}, \quad E_\alpha = L_{12}, \quad E_\beta = L_{1\overline{2}}, \quad E_\gamma = \tfrac{1}{2}L_{1\overline{1}}, \quad E_\delta = \tfrac{1}{2}L_{2\overline{2}} \ . \tag{5-152}$$

The operators $E_{\overline{\alpha}}, E_{\overline{\beta}}, E_{\overline{\gamma}}, E_{\overline{\delta}}$, are obtained from $E_\alpha, E_\beta, E_\gamma, E_\delta$ by interchanging the subscripts of L. These operators differ from those in (5-147) by only multiplicative factors.

2. The complex symplectic group $Sp(2n, C)$.

The infinitesimal matrix $\mathcal{A}(a)$ of $Sp(2n,C)$ still takes the form of (5-146), but now $\mathcal{A}(a)$ is a complex matrix. The infinitesimal operators can still take the form of (5-147), but the parameters $a_{\alpha\beta}$ are now complex. The infinitesimal group elements are expressed as

$$R(a) = 1 + \sum_{\alpha\beta}{}' a_{\alpha\beta} L_{\alpha\beta} \ . \tag{5-153}$$

The sum runs only over the independent parameters. $Sp(2n,C)$ is of order $r = 2n(2n+1)$.

3. Unitary symplectic group Sp_{2n}

The infinitesimal group elements of Sp_{2n} can be expressed as

$$R(a) = 1 + i\sum_{\alpha\beta}{}' a_{\alpha\beta} L_{\alpha\beta} \ , \tag{5-154}$$

where $L_{\alpha\beta}$ are still given by (5-147) and the parameters $a_{\alpha\beta}$ fulfill the hermitian condition

$$a_{\alpha\beta} = a^*_{\beta\alpha} \ .$$

The infinitesimal matrix takes the form

$$\mathcal{A} = i \begin{pmatrix} \mathcal{A}_1 & \mathcal{A}_2 \\ \mathcal{A}_2^\dagger & -\mathcal{A}_1^* \end{pmatrix} \ , \quad \mathcal{A}_1 = \mathcal{A}_1^\dagger, \ \mathcal{A}_2 = \tilde{\mathcal{A}}_2 \ , \tag{5-155}$$

with order $r = n(2n+1)$ and rank $l = n$. As an example, for the group Sp_4, we have

$$\mathcal{A} = i \begin{pmatrix} e_1 & \alpha & \gamma & \beta \\ \alpha^* & e_2 & \beta & \delta \\ \gamma^* & \beta^* & -e_1 & -\alpha^* \\ \beta^* & \delta^* & -\alpha & -e_2 \end{pmatrix} \ , \tag{5-156a}$$

where e_1, e_2 are real and $\alpha, \beta, \gamma, \delta$ are complex. The infinitesimal operators of Sp_4 are

$$H_1, \ H_2, \ (E_\rho + E_{\overline{\rho}}), \quad i(E_\rho + E_{\overline{\rho}}), \quad \rho = \alpha, \beta, \gamma, \delta \ , \tag{5-156b}$$

where $H_1, H_2, E_\alpha, E_{\overline{\alpha}}, \ldots$ are given by (5-152).

The symplectic groups $Sp(2n,C), Sp(2n,R)$ and Sp_{2n} all belong to the classical group C_n.

Ex. 5.1. If the invariant of SO_n is chosen as $\Sigma_{i=-[\frac{n}{2}]}^{[\frac{n}{2}]} x^i x^{-i}$, show that the SO_n generators are given by

$$X_{ii} = 0, \quad X_{ik} = -X_{ki} = c_i^\dagger c_{-k} - c_k^\dagger c_{-i} \ ,$$
$$i \neq k = \begin{cases} 0, \pm 1, \pm 2, \ldots \pm l \\ \pm 1, \pm 2, \ldots \pm 2 \end{cases} \ , \quad \text{for } n = \begin{cases} \text{odd} \\ \text{even} \end{cases} \ ,$$

and that they satisfy the commutators

$$[X_{ik}, X_{mn}] = \delta_{k+m} X_{in} - \delta_{k+n} X_{im} + \delta_{i+n} X_{km} - \delta_{i+m} X_{kn} \ .$$

Ex. 5.2. Show that the generators of Sp_{2n} can be chosen as

$$X_{ik} = X_{ki} = \delta_i c_i^\dagger c_{-k} + \delta_k c_k^\dagger c_{-i} \ ,$$

where $\delta_i = \text{sign } (i)$ and that they satisfy the commutators

$$[X_{ik}, X_{mn}] = \delta_m \delta_{k+m} X_{in} + \delta_n \delta_{k+n} X_{im} + \delta_m \delta_{i+m} X_{kn} + \delta_n \delta_{i+n} X_{km} \ .$$

5.9. The Groups U_{2j+1}, SO_{2l+1} and Sp_{2j+1} .

In Secs. 5.7–5.8, we expressed the generators of the unitary groups and other groups in terms of the creation and annihilation operators in the first quantized formalism. In this section, we re–express the generators using the second quantized formalism.

For physical applications it is convenient to use the generators of the unitary, orthogonal and symplectic groups in the coupled angular momentum form. We use a to denote the angular momentum of single–particle states in a space V, where a can be integer l or half–integer j. The $N = 2a + 1$ single–particle states $\varphi_{a\alpha} \equiv \varphi_\alpha$, $\alpha = a, a-1, \ldots, -a$ carry the defining rep of U_N, SO_N or Sp_N. There are three possible forms for the U_N generators in the coupled form.

Form 1. In the first quantized formalism.

The generators of U_N can be expressed in terms *unit tensor operators* u^r_μ of Racah (1943), or in terms of the tensor operators $p^r = \sqrt{2r+1}u^r$. These operators are defined by specifying their reduced matrix elements in Edmond's convention,

$$\langle a\|u^r\|a\rangle_{\rm Ed} = 1 \ , \quad \langle a\|p^r\|a\rangle_{\rm Ed} = \hat{r} \ , \quad \hat{r} = \sqrt{2r+1} \ . \tag{5-157a}$$

The tensor operator p^r for the i–th particle can be expressed as

$$p^r_{i,\mu} \equiv p^r_i = \left[c^\dagger_a(i)\tilde{c}_a(i)\right]^r_\mu = \sum_{\alpha\beta} C^{r\ \mu}_{a\alpha,a\beta} c^\dagger_\alpha(i)\tilde{c}_\beta(i) \ , \tag{5-157b}$$

where the operator for the time reversed state is defined as

$$\tilde{c}_\beta = (-1)^{a+\beta} c_{-\beta} \ .$$

In the following we often ignore the component index μ.

The generators of U_N for a system with n particles is

$$P^r = \sum_{i=1}^{n} p^r_i \ , \quad r = 0, 1, \ldots, 2a \ . \tag{5-157c}$$

The Cartan subalgebra consists of the operators

$$P^r_0 = \sum_\alpha (-1)^{a-\alpha} C^{r\ 0}_{a\alpha,a-\alpha} \hat{n}_\alpha \ , \quad \hat{n}_\alpha = \sum_{i=1}^{n} c^\dagger_\alpha(i) c_\alpha(i) \ . \tag{5-157d}$$

The matrix representation of p^r_μ is given by

$$U^{(r\mu)}_{\alpha\beta} = \langle a\alpha|p^r_\mu|a\beta\rangle = (-1)^{a-\beta} C^{r\ \mu}_{a\alpha,a-\beta} \ ,$$

where those matrices satisfy

$$\text{Trace } U^{(r\mu)} = \sum_\alpha (-1)^{a-\alpha} C^{r\ \mu}_{a\alpha,a-\alpha} = \hat{a}\delta_{r0}\delta_{\mu 0} \ , \tag{5-158a}$$

showing that except for p^0 all the operators p^r are traceless. Therefore the generators of SU_N are $\{P^r : r = 1, 2, \ldots, 2a\}$.

Racah (1943, 1949), Edmonds & Flowers (1952) and Bayman (1960) use the first quantization formalism to derive the commutators of the generators and of the Casimir operators. We will see that it is much easier to derive those relations in the second quantized formalism.

Form 2. In the second quantized formalism.

Case (i): When V is the total space.

The creation and annihilation operators $C^\dagger_{a\alpha} \equiv C^\dagger_\alpha$ and $C_{a\alpha} \equiv C_\alpha$ obey the commutators

$$C^\dagger_\alpha C^\dagger_\beta \pm C^\dagger_\beta C^\dagger_\alpha = 0 \,,$$

$$C_\alpha C^\dagger_\beta \pm C^\dagger_\beta C_\alpha = \delta_{\alpha\beta} \,, \tag{5-158b}$$

where the plus sign is for fermions ($a = j$) and the minus sign for bosons ($a = l$). The N^2 generators of U_N in the uncoupled form are,

$$E_{\alpha\beta} = C^\dagger_\alpha C_\beta \,, \quad \alpha, \beta = a, a-1, \ldots, -a \,.$$

Using the Wigner–Eckart Theorem we find the second quantized form for a one–body operator T^r of rank r to be

$$\begin{aligned} T^r_\mu &= \sum_{\alpha\beta} \langle a\alpha | T^r_\mu | a\beta \rangle C^\dagger_\alpha C_\beta \\ &= \sum_{\alpha\beta} C^{a\ \alpha}_{a\beta, r\mu} \frac{1}{\hat{a}} \langle a \| T^r \| a \rangle_{\mathrm{Ed}} C^\dagger_\alpha C_\beta \\ &= \frac{1}{\hat{r}} \langle a \| T^r \| a \rangle_{\mathrm{Ed}} \left[C^\dagger_a \tilde{C}_a \right]^r_\mu \,. \end{aligned} \tag{5-159a}$$

From (5-157a) and (5-159a) we get the coupled form of the *generators* of U_N

$$P^r_\mu = \left[C^\dagger_a \tilde{C}_a \right]^r_\mu \,, \quad r = 0, 1, \ldots, 2a \,. \tag{5-159b}$$

Notice that P^0 is related to the number operator $\hat{n}$,

$$P^0 = \frac{\hat{n}}{\sqrt{2a+1}} \,, \qquad \hat{n} = \sum_\alpha \hat{n}_\alpha = \sum_\alpha C^\dagger_\alpha C_\alpha \,. \tag{5-159c}$$

The $N^2 - 1$ generators of SU_N in the uncoupled form are,

$$E_{\alpha\beta} \,, \ \alpha \neq \beta = a, a-1, \ldots, -a; \quad P^r_0, \ r = 1, 2, \ldots, 2a \,. \tag{5-160}$$

Form 3. In the second quantized formalism.

Case (ii): When V is a partial space.

We now assume that V is the orbital space for $a = l$, or the spin–orbital space for $a = j$. The creation operator in the total space is $C^\dagger_{a\alpha\frac{1}{2}\nu} \equiv C^\dagger_{\alpha\nu}$, where $\frac{1}{2}$ is the spin s for integer $a = l$ and isospin t for half–integer $a = j$.

Let us first find the second quantized expression for the operator P^r_μ which acts only in the partial space V. Similar to the derivation of (5-159a) we have

$$\begin{aligned} P^r_\mu &= \sum_{\alpha\beta} \langle a\alpha, t\nu | p^r_\mu | a\beta, t\nu \rangle C^\dagger_{\alpha\nu} C_{\beta\nu} \\ &= \sum_{\alpha\beta} C^{a\ \alpha}_{a\beta, r\mu} \frac{1}{\hat{a}} \langle a \| p^r \| a \rangle_{\mathrm{Ed}} C^\dagger_{\alpha\nu} C_{\beta\nu} \\ &= \sqrt{\frac{2t+1}{2r+1}} \langle a \| p^r \| a \rangle_{\mathrm{Ed}} \left[C^\dagger_{at} \tilde{C}_{at} \right]^{r0}_{\mu 0} \,. \end{aligned} \tag{5-161a}$$

An operator Q^r acting on the isospin space is

$$Q^r_\mu = \sqrt{\frac{2a+1}{2r+1}} \langle t \| q^r \| t \rangle_{\mathrm{Ed}} \left[C^\dagger_{at} \tilde{C}_{at} \right]^{0r}_{0\mu} \,. \tag{5-161b}$$

From (5-157a) and (5-161a) we have

$$\mathbf{P}^r_\mu = \sqrt{2}\left[C^\dagger_{a\frac{1}{2}}\tilde{C}_{a\frac{1}{2}}\right]^{r0}_{\mu 0}, \tag{5-161c}$$

where we used the notation $\mathbf{P}^r_\mu$ for the second quantized expression of generators of U_N to distinguish it from the generators in (5-159b).

To calculate the commutators for the generators of U_N in the coupled basis, it is very convenient to use the technique introduced in Chen, Chen & Klein (1993), by which the commutator of coupled operators can be calculated without using Clebsch–Gordan coefficients. In accordance with Chen, Chen & Klein (1993) the following notation is used: A, B, C, D are operators with angular momentum a, b, c and d respectively. For an operator A one defines $\theta_a = (-1)^{2a} = 1(-1)$ if the operator is bosonic (fermionic). The symbol $(AB)^e_\epsilon$ denotes an operator constructed by angular momentum coupling two operators to a total angular momentum e and z component ϵ, thus

$$(AB)^e_\epsilon = \sum_{\alpha\beta} C^{e\ \epsilon}_{a\alpha,b\beta} A_\alpha B_\beta \ . \tag{5-162a}$$

A commutator with definite angular momentum e and z component ϵ is defined as

$$[A, B]^e_\epsilon = \sum_{\alpha\beta} C^{e\ \epsilon}_{a\alpha,b\beta}(A_\alpha B_\beta - B_\beta A_\alpha) \ . \tag{5-162b}$$

When both A and B are fermionic, the commutator $[A, B]$ should be replaced by the anti-commutator $\{A, B\} = AB + BA$. The basic commutator for two fermions or two bosons is

$$\left[\tilde{C}_a, C^\dagger_b\right]^e_\pm = -[C^\dagger_b, \tilde{C}_a]^e_\pm = \theta_a \delta_{ab}\delta_{e0}\hat{a} \ . \tag{5-162c}$$

From equations (32b), (6) and (25) of Chen, Chen & Klein (1993), we have

$$[P^r, P^s]^t = \hat{r}\hat{s}(-1)^t\left[1 - (-1)^{r+s+t}\right]\begin{Bmatrix} r & s & t \\ a & a & a \end{Bmatrix} P^t \ , \tag{5-163a}$$

$$\begin{aligned}[(A \times B)^e, C]^d_\pm = &\sum_f \hat{e}\hat{f} W(abcd; ef)\left(A \times [B, C]^f_\pm\right)^d \\ &+ \theta_{BC}\sum_f (-1)^{e+f-a-d}\hat{e}\hat{f} W(abdc; ef)\left([A, C]^f_\pm \times B\right)^d \ ,\end{aligned} \tag{5-163b}$$

$$[(A \times B)^0, C] = \sum_f \frac{\hat{f}}{\hat{a}\hat{c}}\left[\theta_{BC}\left([A, C]^f \times B\right)^c + (-1)^{f-a-c}\left(A \times [B, C]^f\right)^c\right] \ , \tag{5-163c}$$

$$\begin{aligned}[(AB)^e \times (CD)^e]^0 = &\theta_{BC}\sum_f \hat{e}\hat{f}(-1)^{e+f-a-d} W(abcd; ef)\left[(AC)^f \times (BD)^f\right]^0 \\ &+ (-1)^{a+b-e}\delta_{bc}\delta_{ad}\frac{\hat{e}}{\hat{a}\hat{b}}[B, C]^0 \times (AD)^0 \ ,\end{aligned} \tag{5-163d}$$

where $\{\ \}$ is a $6j$ symbols (Edmonds 1957), and θ_{BC} equals -1 if both B and C are fermionic, and 1 otherwise.

Notice that Eq. (5-163a) still holds when the single-particle state is labelled by multiple angular momenta, with the replacement $a \to aa'$ (for example $a = j$ and $a' = t$),

$$\begin{aligned}\left[(C^\dagger_{aa'}\tilde{C}_{aa'})^{rr'}, (C^\dagger_{aa'}\tilde{C}_{aa'})^{ss'}\right]^{tt'} = &\hat{r}\hat{r}'\hat{s}\hat{s}'(-1)^{t+t'}\left[1 - (-1)^{(r+s+t)(r'+s'+t')}\right] \\ &\times \begin{Bmatrix} r & s & t \\ a & a & a \end{Bmatrix}\begin{Bmatrix} r' & s' & t' \\ a' & a' & a' \end{Bmatrix}(C^\dagger_{aa'}\tilde{C}_{aa'})^{tt'} \ ,\end{aligned} \tag{5-164}$$

where

$$(C^{\dagger}_{aa'}\tilde{C}_{aa'})^{rr'} = \sum_{\alpha\beta\alpha'\beta'} C^{r\ \mu}_{a\alpha,a\beta} C^{r'\ \mu'}_{a'\alpha',a'\beta'} C^{\dagger}_{\alpha a'} (-1)^{a+a'+\beta+\beta'} C_{-\beta-\beta'} \ .$$

Using (5-164) it can be shown that the commutators between the operators $\{\mathbf{P}^r\}$ are the same as between the operators $\{P^r\}$. Therefore as far as finding the commutators of the generators and the Casimir operators of the groups U_N, Sp_N, SO_N is concerned, we can still use P^r in (5-159b) as the generators for the general case (Case ii). Obviously to work with $\{P^r\}$ is much simpler than with $\{\mathbf{P}^r\}$. The distinction between Case(i) and Case (ii) is that for the former all the irreps of U_N or G_N are one-dimensional, being either totally symmetric (for $a = l$) or totally anti-symmetric (for $a = j$).

From (5-163a) it is seen that the set of operators P^r with $r =$ odd is closed under commutation, and they are the *generators* of SO_N for $a = l$ and of Sp_N for $a = j$. The groups SO_N and Sp_N with $N = 2a + 1$ can be treated in a unified way, designating them together as G_N,

$$G_N (= SO_N \text{ or } Sp_N) =: \{P^r : \ r \text{ odd } \} \ . \tag{5-165}$$

We now show that the invariant (scalar operator) of G_N is a pair of particles coupled to zero angular momentum, called the $\mathcal{S}$ pair,

$$\mathcal{S}^{\dagger} = \sqrt{\frac{2a+1}{2}} (C^{\dagger}_a C^{\dagger}_a)^0 \ . \tag{5-166a}$$

Using (5-163) and (5-162c) we find

$$[\mathcal{S}^{\dagger}, P^r] = \sqrt{2} (C^{\dagger}_a C^{\dagger}_a)^r \ . \tag{5-166b}$$

Since $(C^{\dagger}_a \tilde{C}^{\dagger}_a)^r = 0$ when r is odd, for either fermions or bosons,

$$[G_N, \mathcal{S}^{\dagger}] = 0 \ , \tag{5-167}$$

so that the $\mathcal{S}$ pair is an invariant of G_N.

From the coupled form of the generators P^r of G_N we can easily find the generators in the uncoupled form,

$$P^r_{\mu} = \frac{1}{2} \sum_{\alpha\beta} C^{r\ \mu}_{a\alpha,a\beta} \left(C^{\dagger}_{\alpha} \tilde{C}_{\beta} + (-1)^r \theta_a C^{\dagger}_{\beta} \tilde{C}_{\alpha} \right) \ , \tag{5-168a}$$

$$\theta_a = (-1)^{2a} \ . \tag{5-168b}$$

Therefore the generators of G_N in the uncoupled basis can be taken as $C^{\dagger}_{\alpha} \tilde{C}_{\beta} - \theta_a C^{\dagger}_{\beta} \tilde{C}_{\alpha}$, or

$$X_{\alpha\beta} = (1 + \delta_{\alpha-\beta})^{-1/2} \left(C^{\dagger}_{\alpha} C_{\beta} - (-1)^{\alpha-\beta} C^{\dagger}_{-\beta} C_{-\alpha} \right) \ . \tag{5-169}$$

Equation (5-169) is to be compared with (5-142) and (5-147). From (5-169) we have

$$\begin{aligned} X_{\alpha-\alpha} &= \frac{(1-\theta_a)}{\sqrt{2}} C^{\dagger}_{\alpha} C_{-\alpha} \ , \\ X_{\alpha\alpha} &= H_{\alpha} = n_{\alpha} - n_{-\alpha} \ , \\ X_{\alpha\beta} &= X^{\dagger}_{\beta\alpha} = -\theta_a (-1)^{\alpha+\beta} X_{-\beta-\alpha} \ . \end{aligned} \tag{5-170a}$$

The possible values of $\alpha\beta$ are

$$SO_{2l+1} : \ (\alpha\alpha), \ (\alpha : \alpha - i), \quad \alpha = l, l-1, \ldots, 1; \ i = 1, 2, \ldots 2\alpha - 1 \ , \tag{5-170b}$$

$$Sp_{2j+1}:\ (\alpha\alpha),(\alpha:-\alpha),\ (\alpha:\alpha-i),\quad \alpha=j,j-1,\ldots,\tfrac{1}{2};\ i=1,\ldots 2j-1\ , \tag{5-170c}$$

where $(\alpha:\beta)$ is the abbreviation for $(\alpha\beta),(\beta\alpha)$.

For example, letting $a=1$ we get the generators of SO_3 in the spherical basis,

$$X_{11}=L_0=n_1-n_{-1}\ ,\quad X_{10}=L_+=C_1^\dagger C_0+C_0^\dagger C_{-1}\ ,\quad X_{01}=L_-=C_0^\dagger C_1+C_{-1}^\dagger C_0\ .$$

$$L_0=\begin{pmatrix}1&&\\&0&\\&&-1\end{pmatrix}\ ,\quad L_+=L_-^\dagger=\begin{pmatrix}0&1&0\\0&0&1\\0&0&0\end{pmatrix}\ . \tag{5-171}$$

Those generators obey the commutators

$$[L_+,L_-]=L_0\ ,\quad [L_0,L_\pm]=\pm L_\pm\ .$$

The operator L_0 forms a subalgebra of the Lie algebra (L_+,L_-,L_0).

For $a>1$, the group G_N has the subgroup SO_3 with the generators

$$J_\mu=\sqrt{\frac{a(a+1)(2a+1)}{3}}P_\mu^1\ , \tag{5-172}$$

where Eq. (5-159a) and $\langle a\|J\|a\rangle_{\rm Ed}=\sqrt{a(a+1)(2a+1)}$ have been used.

5.10. Infinitesimal Operators in Group Parameter Space

We use $u(R_a)$ or $u(a)$ to designate functions on the group manifold. The action of Lie group elements on $u(R_a)$ is still defined by (2-87), namely

$$R_b^{-1}u(R_a)=u(R_bR_a)\ . \tag{5-173}$$

Let R_b be an infinitesimal element

$$R_b=R(\delta a)=1+\delta a^\rho X_\rho(a)\ ,$$

$$R_b^{-1}=R^{-1}(\delta a)=1-\delta a^\rho X_\rho(a)\ , \tag{5-174}$$

$$R_bR_a=R(\delta a)R(a)=R(a+da)\ . \tag{5-175}$$

According to the combination law (5-23), we have

$$\begin{aligned}&a^\sigma+da^\sigma=\varphi^\sigma(a,\delta a)\ ,\\ &da^\sigma=\mu_\rho^\sigma(a)\delta a^\rho\ ,\\ &\mu_\rho^\sigma(a)=\frac{\partial\varphi^\sigma(a,b)}{\partial b^\rho}\Big|_{b=0}\ .\end{aligned} \tag{5-176}$$

Rewriting $u(R_a)$ and $u(R_bR_a)$ in (5-173) as $u(a)$ and $u(a+da)$, respectively, and using (5-173), (5-174) and (5-176), we obtain

$$\big(1-\delta a^\rho X_\rho(a)\big)u(a)=u(a+da)=u(a)+\frac{\partial u(a)}{\partial a^\sigma}da^\sigma=u(a)+\frac{\partial u(a)}{\partial a^\sigma}\mu_\rho^\sigma(a)\delta a^\rho\ .$$

Since the δa^ρ are independent, it follows that

$$X_\rho(a)u(a)=-\mu_\rho^\sigma(a)\frac{\partial}{\partial a^\sigma}u(a)\ . \tag{5-177a}$$

Therefore the infinitesimal operators X_ρ in group parameter space are the differential operators

$$X_\rho(a)=-\mu_\rho^\sigma(a)\frac{\partial}{\partial a^\sigma}\ . \tag{5-177b}$$

Racah (1951) and Eisenhart (1933) called $A_\rho(a) = -X_\rho(a)$ the infinitesimal operators of the first parameter group. We use the same name for $X_\rho(a)$.

A simple method for obtaining the infinitesimal operators of the first parameter group was given by Xu (1986) based on the generating coordinate method (GCM).

Example: The infinitesimal operator of SO_2. SO_2 is a one-parameter Abelian group. Let $R(\varphi_c) = R(\varphi_b)R(\varphi_a)$; then $\varphi_c = \varphi_a + \varphi_b$. From (5-177b) and (5-176c) we obtain the infinitesimal operators

$$X_\varphi = -\frac{\partial(\varphi_a + \varphi_b)}{\partial \varphi_b}\frac{\partial}{\partial \varphi} = -\frac{\partial}{\partial \varphi} .$$

Letting $X = -iJ_z$, we have

$$J_z = \frac{1}{i}\frac{\partial}{\partial \varphi} . \tag{5-177c}$$

The infinitesimal operators of SO_3 are calculated, using this approach, in Sec 6.1.

5.11. Isomorphism and Anti-Isomorphism of Lie Groups and Lie Algebras

The Lie algebras $\{X_\rho\}$ and $\{Y_\rho\}$ are said to be *isomorphic* if they are in one-to-one correspondence and have the same structure constants :

$$[X_\rho, X_\sigma] = C^\tau_{\rho\sigma} X_\tau , \tag{5-178a}$$

$$[Y_\rho, Y_\sigma] = C^\tau_{\rho\sigma} Y_\tau . \tag{5-178b}$$

Theorem 5.2: Two Lie groups are locally isomorphic in the neighborhood of the identity and are homomorphic globally, if their Lie algebras are isomorphic :.

For example, the Lie algebra $\{\sigma_x/2, \sigma_y/2, \sigma_z/2\}$ of SU_2 is isomorphic to the Lie algebra $\{J_x, J_y, J_z\}$ of SO_3; thus the Lie groups SU_2 and SO_3 are locally isomorphic in the neighborhood of the identity.

We are going to study the behavior of the groups SO_3 and SU_2 over the whole range of their parameters. With the help of the Pauli matrices in (5-122), we get the matrix representative of the operator $\boldsymbol{\sigma}\cdot\mathbf{n}$ in the basis $\binom{1}{0}, \binom{0}{1}$, which are eigenfunctions of σ_z,

$$\boldsymbol{\sigma}\cdot\mathbf{n} = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta \end{pmatrix} , \tag{5-179a}$$

where θ and φ are the orientation angles of $\mathbf{n}$. The eigenfunctions of $\boldsymbol{\sigma}\cdot\mathbf{n}$ are

$$\chi_{\frac{1}{2}} = \begin{pmatrix} \cos\frac{\theta}{2}e^{-\frac{i}{2}\varphi} \\ \sin\frac{\theta}{2}e^{\frac{i}{2}\varphi} \end{pmatrix} , \quad \chi_{-\frac{1}{2}} = \begin{pmatrix} -\sin\frac{\theta}{2}e^{-\frac{i}{2}\varphi} \\ \cos\frac{\theta}{2}e^{\frac{i}{2}\varphi} \end{pmatrix} . \tag{5-179b}$$

Under the SU_2 transformation [(5-29)], the spin wave functions and the operator $\boldsymbol{\sigma}\cdot\mathbf{n}$ transform as follows

$$\begin{pmatrix} a \\ b \end{pmatrix} \to \begin{pmatrix} a' \\ b' \end{pmatrix} = U\begin{pmatrix} a \\ b \end{pmatrix} , \tag{5-180a}$$

$$(\boldsymbol{\sigma}\cdot\mathbf{n}) \to (\boldsymbol{\sigma}\cdot\mathbf{n})' = U(\boldsymbol{\sigma}\cdot\mathbf{n})U^{-1} . \tag{5-180b}$$

The most general form of the transformation matrix of SU_2 is given by (5-29). Putting $\xi = \alpha/2, \eta = \xi = 0$, we have

$$U = A_z(\alpha) = \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix} . \tag{5-181}$$

According to (5-179) and (5-181), we have

$$(\boldsymbol{\sigma}\cdot\mathbf{n})' = \boldsymbol{\sigma}\cdot\mathbf{n}' = \begin{pmatrix} \cos\theta & \sin\theta e^{-i(\varphi+\alpha)} \\ \sin\theta e^{i(\varphi+\alpha)} & -\cos\theta \end{pmatrix} . \tag{5-182}$$

$$\chi'_{\frac{1}{2}} = \begin{pmatrix} \cos\frac{\theta}{2}\cdot e^{-\frac{i}{2}(\varphi+\alpha)} \\ \sin\frac{\theta}{2}\cdot e^{\frac{i}{2}(\varphi+\alpha)} \end{pmatrix} , \quad \chi'_{-\frac{1}{2}} = \begin{pmatrix} -\sin\frac{\theta}{2}\cdot e^{-\frac{i}{2}(\varphi+\alpha)} \\ \cos\frac{\theta}{2}\cdot e^{\frac{i}{2}(\varphi+\alpha)} \end{pmatrix} . \tag{5-183}$$

Evidently, $\chi'_{\pm\frac{1}{2}}$ are eigenfunctions of $\boldsymbol{\sigma}\cdot\mathbf{n}'$. Thus the effect of the SU_2 transformation (5-181) on the operator $\boldsymbol{\sigma}\cdot\mathbf{n}$ is equivalent to rotating the unit vector $\mathbf{n}$ through angle α about the z-axis in three-dimensional space. Therefore the SU_2 matrix $A_z(\alpha)$ of (5-181) corresponds to the SO_3 matrix $R_z(\alpha)$ of (5-30b).

Analogously, in (5-29), by putting $\xi = \zeta = 0, \eta = \beta/2$, we have

$$U = A_y(\beta) = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} . \tag{5-184}$$

For simplicity, we let $\varphi = 0$ in (5-179), that is, let $\mathbf{n}$ be in the x-z plane. From (5-179), (5-180) and (5-184) we obtain

$$\boldsymbol{\sigma}\cdot\mathbf{n} = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \to \boldsymbol{\sigma}\cdot\mathbf{n}' = \begin{pmatrix} \cos(\theta+\beta) & \sin(\theta+\beta) \\ \sin(\theta+\beta) & -\cos(\theta+\beta) \end{pmatrix} , \tag{5-185}$$

$$\chi_{\frac{1}{2}} = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} \to \chi'_{\frac{1}{2}} = \begin{pmatrix} \cos\left(\frac{\theta+\beta}{2}\right) \\ \sin\left(\frac{\theta+\beta}{2}\right) \end{pmatrix} , \tag{5-186}$$

$$\chi_{-\frac{1}{2}} = \begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix} \to \chi'_{-\frac{1}{2}} = \begin{pmatrix} -\sin\left(\frac{\theta+\beta}{2}\right) \\ \cos\left(\frac{\theta+\beta}{2}\right) \end{pmatrix} . \tag{5-187}$$

It follows that the SU_2 transformation $A_y(\beta)$ of (5-184) corresponds to the rotation $R_y(\beta)$ (5-32). In summary, the SU_2 matrix which corresponds to the three-dimensional rotation matrix $\mathcal{D}(\alpha\beta\gamma) = R_z(\alpha)R_y(\beta)R_z(\gamma)$ is equal to

$$D^{\frac{1}{2}}(\alpha\beta\gamma) = A_z(\alpha)A_y(\beta)A_z(\gamma) = \begin{pmatrix} e^{-\frac{i}{2}(\alpha+\gamma)}\cos\frac{\beta}{2} & -e^{-\frac{i}{2}(\alpha-\gamma)}\sin\frac{\beta}{2} \\ e^{\frac{i}{2}(\alpha-\gamma)}\sin\frac{\beta}{2} & e^{\frac{i}{2}(\alpha+\gamma)}\cos\frac{\beta}{2} \end{pmatrix} . \tag{5-188}$$

In fact it is just the $j = 1/2$ representation matrix of SO_3 (Rose 1957).

Moreover, it is easy to prove that if the SU_2 matrices A and B correspond to the rotation matrices R_A and R_B, respectively, then the product AB corresponds to R_AR_B. The proof is as follows:

$$A(\boldsymbol{\sigma}\cdot\mathbf{n})A^{-1} = \boldsymbol{\sigma}\cdot R_A\mathbf{n}, \quad B(\boldsymbol{\sigma}\cdot\mathbf{n})B^{-1} = \boldsymbol{\sigma}\cdot R_B\mathbf{n} ,$$
$$AB(\boldsymbol{\sigma}\cdot\mathbf{n})(AB)^{-1} = AB(\boldsymbol{\sigma}\cdot\mathbf{n})B^{-1}A^{-1} = A(\boldsymbol{\sigma}\cdot R_B\mathbf{n})A^{-1} = \boldsymbol{\sigma}\cdot R_AR_B\mathbf{n} .$$

It must be emphasized that the correspondence between the groups SU_2 and SO_3 is not one-to-one. For example, from (5-181) and (5-32) we see that

$$A_z(\alpha+2\pi) = -A_z(\alpha), \quad R_z(\alpha+2\pi) = R_z(\alpha) . \tag{5-189}$$

Rotations through angle α and $\alpha+2\pi$ about any fixed axis are physically identical. Nevertheless, they correspond to different elements of the group SU_2. Therefore the isomorphism between the Lie algebras of SU_2 and SO_3 only ensures that SU_2 and SO_3 group are isomorphic in the neighborhood of the identity. They are homomorphic over the whole range of parameters.

The rotation group can be generalized in the following way: we will distinguish the rotation through angle α and $\alpha+2\pi$ about an axis, but not distinguish the rotations through angle α

and $\alpha + 4\pi$. The generalized rotation group is called the *double rotation group*, denoted $SO_3^\dagger$. There is a one-to-one correspondence between the elements of SU_2 and $SO_3^\dagger$. Now each matrix of SU_2 corresponds uniquely to a "rotation" of $SO_3^\dagger$. $SO_3^\dagger$ is isomorphic to SU_2 and SU_2 is called the *universal covering group* of SO_3.

We thus see that the rotation matrices form an unfaithful rep of SU_2, and the homomorphism of SU_2 on SO_3 has Z_2 as its kernel. Conversely, any element of SO_3 can be represented by an SU_2 matrix up to sign. Therefore, in general, SU_2 reps are projective reps of SO_3. We can also say that the matrices of SU_2 form a *double-valued rep* of SO_3.

Each SO_n group has a universal covering group, called the *spin group* . For SO_3, as we have said it is SU_2; for SO_4, it is the group $SU_2 \times SU_2$; for SO_5 and SO_6, they are Sp_4 and SU_4 respectively.

The importance of the universal covering group is that all the reps of a group G can be found from a study of the single-valued reps of its universal covering group.

In summary we have the following isomorphism for compact Lie groups.

$$SO_3 \approx SU_2/Z_2, \quad SO_4 \approx [SU_2 \times SU_2]/Z_2 \ ,$$
$$SO_5 \approx Sp_4/Z_2, \quad SO_6 \approx SU_4/Z_2 \ .$$

The Lie algebras $\{X_\rho\}$ and $\{Z_\rho\}$ are said to be anti-isomorphic if they are in one-to-one correspondence and that if the X_ρ satisfy (5-178a), then the corresponding commutation relation for the Z_ρ is

$$[Z_\rho, Z_\sigma] = -C^\tau_{\rho\sigma} Z_\tau \ . \tag{5-190}$$

Two Lie groups are locally anti-isomorphic in the neighborhood of the identity if their Lie algebras are anti-isomorphic. Thus, if $R(a)$ and $S(a)$ are the elements of the Lie groups generated by $\{X_\rho\}$ and $\{Z_\rho\}$, then in the neighborhood of the identity corresponding to

$$R(a)R(b) = R(c) \ ,$$

we have

$$S(b)S(a) = S(c) \ . \tag{5-191}$$

Clearly, if $\{Z_\rho\}$ is anti-isomorphic to $\{X_\rho\}$, then $\{-Z_\rho\}$ is isomorphic to $\{X_\rho\}$.

5.12. Invariant Integration

In the derivation of theorems for finite groups, we often used the following property

$$\sum_{a=1}^{g} u(R_a) = \sum_{a=1}^{g} u(R_b^{-1} R_a) \ , \tag{5-192}$$

where R_b is a definite element. (5-192) implies that we attached equal weights to all elements R of a finite group (see (2.73)).

To extend the theorems of finite groups to Lie groups, (5-192) must be expressed as an integral over the group parameters a. For this purpose, we have to introduce the *Density function* $\rho(a) = \rho(a^1, a^2, \ldots, a^r)$, depending on the r parameters of the Lie group and demand that the integral of the function $u(R_a)$ over the whole domain of the r parameters be invariant under the following parameter transformations

$$\int_G u(R_a)\rho(a)da = \int_G u(R_b^{-1}R_a)\rho(a)da = \int_G u(R_a R_b^{-1})\rho(a)da \ , \tag{5-193}$$
$$da = da^1 da^2 \ldots da^r \ .$$

It can be proved that for compact Lie groups we can always find such density functions (Hamermesh 1962). The density function is also called the *weight function.*

The definition of scalar product for functions on the group manifold can be generalized from (2-84)

$$\langle u_1|u_2\rangle = \sum_a u_1^*(R_a)u_2(R_a) \tag{5-194}$$

to

$$\langle u_1|u_2\rangle = \int_G u_1^*(a)u_2(a)\rho(a)da\ . \tag{5-195}$$

Weyl proved that the class operator $C(\varphi) = C(\varphi^1, \varphi^2, \ldots, \varphi^l)$ of a compact Lie group with rank l only depends on l class parameters $\varphi^1, \varphi^2, \ldots, \varphi^l$. $C(\varphi)$ is the weighted integration over all the elements belonging to the same class.

$$C(\varphi) = \int_{R(a')\in C(\varphi)} R(a')\rho(a')da'\ . \tag{5-196}$$

The number of elements, g_i, belonging to the class i is replaced by the volume $g(\varphi)$ occupied by the elements of the class φ in the group parameter space,

$$g(\varphi) = \int_{R(a')\in C(\varphi)} \rho(a')da'\ . \tag{5-197}$$

In the class parameter space, we can analogously define a density function

$$\rho(\varphi) = \rho(\varphi^1, \varphi^2, \ldots, \varphi^l)\ , \tag{5-198}$$

so that the scalar product of functions on classes can be extended from (3-14)

$$\langle q_1|q_2\rangle = \sum_i g_i q_1^*(C_i)q_2(C_i) \tag{5-199}$$

to

$$\begin{gathered}\langle q_1|q_2\rangle = \int g(\varphi)q_1^*(\varphi)q_2(\varphi)\rho(\varphi)d\varphi, \\ d\varphi = d\varphi^1 d\varphi^2 \ldots d\varphi^l\ .\end{gathered} \tag{5-200}$$

The total number of elements of a finite group is replaced by the total *volume of the Lie group*

$$g = \sum_{a=1}^{g} 1 \to g = \int \rho(a)da = \int \rho(\varphi)d\varphi \int \rho(a')da'\ . \tag{5-201}$$

The method for finding the density function $\rho(a)$ is given by Hamermesh (1962). A simpler method for obtaining the density function of SO_3 will be given in Sec. 6.3.

5.13. Representations of Compact Lie groups

The definition of reps of Lie groups is the same as that of finite groups. A rep is said to be reducible if through a similarity transformation all the rep matrices can be brought to the following form,

$$D(R) = \left(\begin{array}{c|c} D^{(1)}(R) & A(R) \\ \hline 0 & D^{(2)}(R) \end{array}\right)\ . \tag{5-202}$$

The rep is said to be fully reducible if all the submatrices $A(R) = 0$. For finite groups, reducible reps are necessarily fully reducible. However reducible reps of Lie groups may not be fully

reducible. For example, under the translation operation $x' = x+a$, the basis functions $\varphi_1(x) = 1$ and $\varphi_2(x) = x$ go over to

$$\begin{pmatrix} \varphi_1'(x) \\ \varphi_2'(x) \end{pmatrix} = \begin{pmatrix} 1 \\ x+a \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ a & 1 \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix} . \tag{5-203a}$$

Thus a rep for the translation group is found to be

$$D(a) = \begin{pmatrix} 1 & a \\ 0 & 1 \end{pmatrix} . \tag{5-203b}$$

The rep $D(a)$ is reducible, but not fully reducible, that is, we cannot find a similarity transformation which will bring $D(a)$ into diagonal form. Only for fully reducible cases can the study of group reps be reduced to that of all the irreps of the group. For semi–simple Lie groups we have Theorem 5.3.

Theorem 5.3 (Weyl's theorem): Any reducible rep of a semi–simple Lie algebra is fully reducible.

For compact Lie groups, all the theorems which were derived for finite groups in Chapter 3 still hold (Hamermesh 1962). For example, every rep of a compact group is equivalent to a unitary rep. Every rep of a compact group is fully reducible to a sum of irreps, all of which have finite dimensions, and the regular rep contains all irreps.

As we have said, the problem of finding reps of a Lie group can be reduced to that of finding reps of the corresponding Lie algebra, namely, finding r matrices $D(X_\rho)$ for the r infinitesimal operators X_ρ so that they obey the Lie algebra relation

$$[D(X_\rho), D(X_\sigma)] = C_{\rho\sigma}^{\tau} D(X_\tau) . \tag{5-204}$$

5.13.1. The fundamental representation

The linear transformations $R(a)$ in n–dimensional space themselves form a rep of the linear transformation group. This n–dimensional rep is called the *fundamental* or *defining rep.*

5.13.2. Adjoint representations

For finite groups, corresponding to each element R_a of a group G, we can define an operator $\overset{\circ}{R}_a$ by

$$\overset{\circ}{R}_a S = R_a S R_a^{-1} = T, \quad S \in G . \tag{5-205}$$

The set of operators $\overset{\circ}{R}_a$ also forms a rep of the group G, known as the *adjoint rep.* Let S be an infinitesimal operator

$$S = 1 + \varepsilon X_\rho . \tag{5-206a}$$

Then the element T in (5-205) is also an infinitesimal operator and can be written as

$$T = 1 + \varepsilon \sum_\sigma \mathcal{D}_{\sigma\rho}^{(\nu_0)}(a) X_\sigma . \tag{5-206b}$$

Substituting (5-206) into (5-205) and noting that $\overset{\circ}{R}(a)e = R(a)eR^{-1}(a) = e$, we obtain

$$\overset{\circ}{R}(a) X_\rho = R(a) X_\rho R^{-1}(a) = \sum_\sigma \mathcal{D}_{\sigma\rho}^{(\nu_0)}(a) X_\sigma . \tag{5-207}$$

This shows that the r infinitesimal operators $X_1, X_2, \ldots, X_r$ carry an r-dimensional rep of the Lie group G, which is called the *adjoint rep* of the Lie group and denoted (ν_0).

Suppose that under a Lie group G the r functions $\psi_\rho^{(\nu_0)}$ transform among themselves according to the adjoint rep $\mathcal{D}^{(\nu_0)}$,

$$R(a)\psi_\rho^{(\nu_0)} = \sum_\sigma \mathcal{D}_{\sigma\rho}^{(\nu_0)}(a)\psi_\sigma^{(\nu_0)} , \tag{5-208a}$$

$$\mathcal{D}_{\sigma\rho}^{(\nu_0)}(a) = \langle \psi_\sigma^{(\nu_0)} | R(a) | \psi_\rho^{(\nu_0)} \rangle \equiv \langle \nu_0 \sigma | R(a) | \nu_0 \rho \rangle . \tag{5-208b}$$

Letting

$$R(a) = 1 + \delta a^\tau X_\tau, \quad \overset{\circ}{R}(a) = 1 + \delta a^\tau \overset{\circ}{X}_\tau , \tag{5-209}$$

Eq. (5-208b) becomes

$$\mathcal{D}_{\sigma\rho}^{(\nu_0)}(a) = \delta_{\sigma\rho} + \delta a^\tau \mathcal{D}_{\sigma\rho}^{(\nu_0)}(X_\tau) , \tag{5-210a}$$

$$\mathcal{D}_{\sigma\rho}^{(\nu_0)}(X_\tau) = \langle \nu_0 \sigma | X_\tau | \nu_0 \rho \rangle . \tag{5-210b}$$

Substituting (5-209) and (5-210) into (5-207), we get

$$\overset{\circ}{X}_\tau X_\rho = [X_\tau, X_\rho] = \sum_\sigma \mathcal{D}_{\sigma\rho}^{(\nu_0)}(X_\tau) X_\sigma . \tag{5-211}$$

$\overset{\circ}{X}_\tau$ is called the *adjoint operator* of X_τ, which transforms an element X_ρ of the algebra into the element $[X_\tau, X_\rho]$.

Comparing (5-211) with (5-43), we obtain the representatives of the infinitesimal operators X_τ in the adjoint rep:

$$\mathcal{D}_{\sigma\rho}^{(\nu_0)}(X_\tau) \equiv D_{\sigma\rho}(\overset{\circ}{X}_\tau) = C_{\tau\rho}^\sigma . \tag{5-212a}$$

Theorem 5.4: The adjoint rep of a simple algebra is irreducible.

Proof: Since, according to Sec. 5.5, a simple Lie algebra $A = \{X_\tau : \tau = 1, 2, \ldots, r\}$ means that among its r infinitesimal operators, we cannot find a subset $A_s = (X_i, X_j, \ldots, X_k), k < r$, such that it is closed under the adjoint operations of the r infinitesimal operators X_τ,

$$\overset{\circ}{X}_\tau X_i \equiv [X_\tau, X_i] \in A_s . \tag{5-212b}$$

If the adjoint rep is reducible, then (5-212b) is true, contradicting the assumption that the Lie algebra is simple. **QED**

Theorem 5.5: The adjoint rep of a semi-simple algebra is faithful.

5.13.3. The metric tensor in the r-dimensional vector space

The r infinitesimal operators $X_\alpha, \alpha = 1, 2, \ldots, r$, can be considered as a covariant basis in the r-dimensional space $\mathcal{L}_r$[1]. The scalar product of any two vectors A and B in $\mathcal{L}_r$ is required to be independent of the original choice of the basis $\{X_\alpha\}$, that is, it must be defined in terms of a matrix invariant. Therefore, the scalar product of two basis vectors X_α and X_β is defined by

$$g_{\alpha\beta} = \langle X_\alpha, X_\beta \rangle = \mathrm{Tr}\left(D(\overset{\circ}{X}_\alpha) D(\overset{\circ}{X}_\beta)\right) = C_{\alpha\rho}^\sigma C_{\beta\sigma}^\rho . \tag{5-213a}$$

[1] Care must be taken to distinguish the r-dimensional space $\mathcal{L}_r$ from the previous n-dimensional space. For example the eight infinitesimal operators of SU_3, $E_{ij} = x^i \frac{\partial}{\partial x^j} - \frac{1}{3}\delta^i_j x^i \frac{\partial}{\partial x^i}, i = 1,2,3$, are the second rank mixed tensor in the ordinary space of dimension n (=3), while in the r (=8)-dimensional space, they are the covariant basis vectors X_α.

The covariant tensor $g_{\alpha\beta}$ of rank two is the *metric tensor in the Lie algebra space* $\mathcal{L}_r$ and is knows as the *Killing form* . Under the basis transformation (5-47a), it becomes

$$g'_{\alpha\beta} = C'^{\sigma}_{\alpha\rho} C'^{\rho}_{\beta\sigma}, \quad g' = BgB^{\sim} . \tag{5-213b}$$

The scalar product of any two vectors $X_A = a^\alpha X_\alpha$ and $X_B = b^\beta X_\beta$ is given by

$$\langle X_A, X_B \rangle = a^\alpha b^\beta \langle X_\alpha, X_\beta \rangle = a^\alpha g_{\alpha\beta} b^\beta . \tag{5-214}$$

Theorem 5.6 (Cartan's Theorem) : The necessary and sufficient condition for a Lie algebra to be semi-simple is that the determinant of the metric tensor g does not vanish,

$$\det|g_{\alpha\beta}| \neq 0 . \tag{5-215}$$

From the structure constants $C^\sigma_{\alpha\rho}$ of a Lie algebra, we can construct g, and from (5-215) we can check whether it is semi-simple or not.

We restrict ourselves to semi-simple groups; therefore from $g_{\alpha\beta}$ we can find the contravariant metric tensor $g^{\alpha\beta}$ by using (5-12a). The matrices $g_{\alpha\beta}$ and $g^{\alpha\beta}$ can be used to lower or raise indices:

$$X^\alpha = g^{\alpha\beta} X_\beta , \quad X_\alpha = g_{\alpha\beta} X^\beta . \tag{5-216}$$

Theorem 5.7: A semi-simple algebra is *compact* if and only if $\det|g_{\alpha\beta}| < 0$.

5.14. The Invariants and Casimir Operators of Lie Groups

If $I(X_\rho)$ is an operator built out of the r infinitesimal operators and if it is invariant under the group G,

$$I(X'_\rho) = I\big(R(a) X_\rho R^{-1}(a)\big) = R(a) I(X_\rho) R^{-1}(a) = I(X_\rho) , \tag{5-217a}$$

namely,

$$[I(X_\rho), R(a)] = 0 , \tag{5-217b}$$

then $I(X_\rho)$ is called an *invariant* of the group G. In other words, $I(X_\rho)$ is a scalar with respect to the group operation.

It can be shown that any invariant must commute with all the infinitesimal operators of G. Assuming that the $R(a)$ in (5-217) are infinitesimal transformations,

$$I(X'_\rho) = \exp(\delta a^\sigma X_\sigma) I(X_\rho) \exp(-\delta a^\tau X_\tau) = I(X_\rho) , \tag{5-218}$$

where δa^σ are infinitesimal quantities. Expanding the exponential functions, we obtain

$$[I(X_\rho), X_\sigma] = 0, \quad \sigma = 1, 2, \ldots, r . \tag{5-219}$$

Conversely, if an operator $I(X_\rho)$ commutes with all the infinitesimal operators, then $I(X_\rho)$ is an invariant of the group G.

With the help of the metric tensor, it is easy to find a quadratic invariant

$$\mathcal{C} = X_\alpha g^{\alpha\beta} X_\beta = X_\alpha X^\alpha , \tag{5-220a}$$

called the Casimir operator. Using (5-43) and (5-44) it can be shown that

$$[\mathcal{C}, X_\sigma] = 0 , \quad \sigma = 1, 2, \ldots, r . \tag{5-220b}$$

One can use tensor contractions to construct higher order invariants. For example

$$C^{(3)} = C^{\beta_2}_{\alpha_1\beta_1} C^{\beta_3}_{\alpha_2\beta_2} C^{\beta_1}_{\alpha_3\beta_3} X^{\alpha_1} X^{\alpha_2} X^{\alpha_3} . \tag{5-220c}$$

Such higher order invariants are called *generalized Casimir operators* .

Apart from the Casimir operators, there are many ways to construct invariants (see Sec. 7.2). It can be shown that for a semi-simple Lie group of rank l, there exist l invariants $I_1(X_\rho), \ldots, I_l(X_\rho)$ (Racah 1951). The set of operators

$$\mathbf{C} = \big(I_1(X_\rho), \ldots, I_l(X_\rho)\big) \tag{5-221a}$$

forms a CSCO in the class parameter space (the CSCO $\mathbf{C}$ is not to be confused with the Casimir operator C). We call this CSCO a *CSCO of the first kind* (CSCO-I) of the Lie group .

Since the class operator $C(\varphi)$ in (5-196) commutes with any elements of a Lie group G, according to Theorem 2.2, $C(\varphi)$ is necessarily a function of the CSCO-I of G,

$$C(\varphi^1, \varphi^2, \ldots, \varphi^l) = f\big(\varphi^1, \varphi^2, \ldots, \varphi^l; I_1, I_2, \ldots, I_l\big) . \tag{5-221b}$$

For examples see (6-11) and (6-27b).

As an example, for the group SO_3 with rank one, there is only one invariant $\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2$. $\mathbf{J}^2$ is the CSCO-I of SO_3.

In physical applications the quadratic Casimir operator is most important, and its multiplicative factor is irrelevant. One often defines a Casimir operator which differs from (5-220a) by a factor and will be designated by C. The *Casimir operators* of U_N, SU_N, SO_N and Sp_N with $N = 2a + 1$ can easily be constructed in terms of the generators P^r in (5-159b)

$$C_{U_N} = \sum_{r=0}^{2a} (-1)^r \hat{r} (P^r \cdot P^r)^0 \equiv \sum_{r=0}^{2a} P^r \cdot P^r \equiv \sum_{r=0}^{2a} \sum_{\mu} (-1)^\mu P^r_\mu P^r_{-\mu}, \tag{5-222a}$$

$$C_{SU_N} = \sum_{r=1}^{2a} P^r \cdot P^r = C_{U_N} - \frac{\hat{n}^2}{N}, \tag{5-222b}$$

where we use (5-159c) in the last step.

Using the orthogonality of the CG coefficients, we can write C_{U_N} in the uncoupled basis as

$$C_{U_N} = \sum_{\alpha\beta} C^\dagger_\alpha C_\beta C^\dagger_\beta C_\alpha . \tag{5-222c}$$

We want to prove that (5-222a) is the Casimir operator of U_N. Using (5-163) and (5-222a) we have

$$[C_{U_N}, P^s] = 2 \sum_{rt} (-1)^{r+t} \hat{r}\hat{t} \Delta_{rst} \begin{Bmatrix} r & s & t \\ a & a & a \end{Bmatrix} \big((P^r \times P^t)^s - (P^t \times P^r)^s\big) = 0, \tag{5-223}$$

$$\Delta_{rst} = \begin{cases} 1, & r+s+t \text{ odd} \\ 0, & \text{otherwise} \end{cases} ,$$

since both the summation indices r, t are from 0 to $2a$, and since the term inside the brackets is anti-symmetric in r and t. Thus (5-222a) is indeed the Casimir operator of U_n.

Since the term $\frac{\hat{n}^2}{N}$ commutes with P^s, we know from (5-223) that Eq. (5-222b) is also the Casimir operator of SU_N.

Similarly, since the set of operators P^r with r = odd is closed under commutation, we know that the Casimir operator of G_N is

$$C_{G_N} = 2 \sum_{r\,\text{odd}} P^r \cdot P^r \ . \tag{5-222d}$$

5.15. Intrinsic Lie Groups

5.15.1. Definition and interpretation of the intrinsic Lie group

For any Lie group $G = \{R(a)\}$ we can define an intrinsic Lie group $\overline{G} = \{\overline{R}(a)\}$ in analogy with the definition for finite groups. The action of the intrinsic group element $\overline{R}(b)$ on any element $R(a)$ in the group space is defined by

$$\overline{R}(b)R(a) = R(a)R(b) \ . \tag{5-224}$$

The groups $\overline{G}$ and G are anti-isomorphic and commute. Thus their corresponding Lie algebras obey

$$[X_\tau, \overline{X}_\rho] = 0 \ , \quad \tau, \rho = 1, 2, \ldots, r \ . \tag{5-225}$$

$$[X_\tau, X_\rho] = C^\sigma_{\tau\rho} X_\sigma \ , \quad [\overline{X}_\tau, \overline{X}_\rho] = -C^\sigma_{\tau\rho} \overline{X}_\sigma \ .$$

From (5-224) we obtain a relation between the intrinsic group element $\overline{R}(b)$ and the group element $R(b)$:

$$\overline{R}(b) = R(a)R(b)R(a)^{-1} \ , \quad \text{when } R(b) \text{ acts on } R(a) \ . \tag{5-226a}$$

It should be emphasized that (5-226a) is the defining equation for the operator $\overline{R}(b)$ rather than an operator identity [see the remarks after (3-144)].

We first prove that (5-226a) holds when $\overline{R}(b)$ acts on any function $u(a)$ on the group manifold, that is

$$\overline{R}(b)u(a) = R(a)R(b)R^{-1}(a)u(a) \ , \tag{5-226b}$$

Proof: According to (3-138), the left-hand side of (5-226b) is

$$\overline{R}(b)u(a) = \overline{R}(b)u\big(R(a)\big) = u\big(R(a)R^{-1}(b)\big) \ , \tag{5-226c}$$

while according to (2-87b), the right-hand side of (5-226b) is

$$R(a)R(b)R^{-1}(a)u(a) = u\Big[\big(R(a)R(b)R^{-1}(a)\big)^{-1}R(a)\Big] = u\big(R(a)R^{-1}(b)\big) \ .$$

Therefore (5-226b) is true. **QED**

Equation (5-226b) is an operator identity in the sense that it holds for any group parameters a and b.

Let $R(b)$ be an infinitesimal element,

$$R(b) = 1 + \delta b^\rho X_\rho \ . \tag{5-226d}$$

Its corresponding intrinsic element is

$$\overline{R}(b) = 1 + \delta b^\rho \overline{X}_\rho \ . \tag{5-226e}$$

When acting on the function $u(a)$, $X_\rho \to X_\rho(a)$ and $\overline{X}_\rho \to \overline{X}_\rho(a)$. The differential operators of $X_\rho(a)$ and $\overline{X}_\rho(a)$ are given by (5-177b) and (5-234), respectively. Inserting (5-226d) and (5-226e) into (5-226b), we obtain

$$\big(1 + \delta b^\rho \overline{X}_\rho(a)\big)u(a) = R(a)\big(1 + \delta b^\rho X_\rho(a)\big)R^{-1}(a)u(a) \ .$$

Since $u(a)$ is an arbitrary function on the group manifold, it follows that

$$\overline{X}_\rho(a) = R(a)X_\rho(a)R^{-1}(a) \ . \tag{5-227}$$

On the other hand, the r infinitesimal operators $\{X_\rho\}$ carry the adjoint rep (ν_0) of the group G. From (5-207) and (5-227) we have

$$\overline{X}_\rho(a) = \sum_\sigma \mathcal{D}^{(\nu_0)}_{\sigma\rho}(a)X_\sigma(a) \ . \tag{5-228a}$$

The inverse of (5-228a) is

$$X_\sigma(a) = \sum_\rho (\mathcal{D}^{(\nu_0)}(a))^{-1}_{\rho\sigma}\overline{X}_\rho(a) \ . \tag{5-228b}$$

Equations (5-228a) and (5-228b) gives the relations between the infinitesimal operators of the Lie group G and the intrinsic Lie group $\overline{G}$. Since the group parameters a in (5-227) and (5-228) are variables, it follows that

$$[X_\rho(a), \mathcal{D}^{(\nu_0)}(a)] \neq 0, \quad [\overline{X}_\rho(a), \mathcal{D}^{(\nu_0)}(a)] \neq 0 \ .$$

[For the explicit form see (5-259) and (5-262)]. If we hold the group parameters a in (5-227) constant at a_0, but leave the algebraic parameter a as a variable, letting $\overline{X}_\rho \to X'_\rho$ gives

$$X'_\rho(a) = R(a_0)X_\rho(a)R^{-1}(a_0) = \sum_\sigma \mathcal{D}^{(\nu_0)}_{\sigma\rho}(a_0)X_\sigma(a) \ . \tag{5-229}$$

Now a_0 are constants and we have

$$[X_\rho(a), \mathcal{D}^{(\nu_0)}(a_0)] = [X'_\rho(a), \mathcal{D}^{(\nu_0)}(a_0)] = 0 \ .$$

It must be stressed that although (5-227) and (5-229) are similar in appearance, they are really very different. To give a geometrical interpretation of (5-229), we consider the r infinitesimal operators X_ρ as components of an abstract vector X in a fixed coordinate system of an r–dimensional space $\mathcal{L}_r$. Then (5-229) shows that $X'(a)$ are the new components of the vector X in another fixed system rotated through a given angle a_0 with respect to the original one. $X'_\rho(a)$ and $X_\rho(a)$ are members of the same Lie algebra. In other words, $\{X'_\rho\}$ and $\{X_\rho\}$ are isomorphic but do not commute.

In contrast to (5-229), (5-227) can be regarded as a transformation from the fixed coordinate system to the moving (or body–fixed, or intrinsic) coordinate system, where the parameters a are variables instead of constants, since the "orientation angles" a of a moving frame with respect to the fixed one are dynamic variables. It is precisely this that makes the Lie algebras $\{X_\rho\}$ and $\{\overline{X}_\rho\}$ commute and be anti–isomorphic. Therefore, the infinitesimal operators $\overline{X}_\rho$ of the intrinsic group $\overline{G}$ can be thought of as the components of the same vector X in the intrinsic frame. These physical interpretations can be more clearly seen in the example for the group SO_3 to be discussed in Sec. 6.1.

Finally, we want to point out that the relation (5-228a) between the infinitesimal operators of the first and second parameter groups is a generalization of Eisenhart's equation (Eisenhart 1933, equation 14.10). For details, see Chen, Wang & Gao (1983).

5.15.2. Infinitesimal operators of intrinsic groups in group parameter space

From (5-226c) we have

$$\overline{R}_b^{-1}u(R_a) = u(R_aR_b) \ . \tag{5-230}$$

In parallel with (5-174)-(5-177) we may write

$$\begin{aligned} R_b &= R(\delta a) = 1 + \delta a^\rho X_\rho(a) \ , \\ \overline{R}_b^{-1} &= \overline{R}^{-1}(\delta a) = 1 - \delta a^\rho \overline{X}_\rho(a) \ , \end{aligned} \tag{5-231}$$

$$\begin{aligned} R_a R_b &= R(a)R(\delta a) = R(a + da) \ , \\ a^\sigma + da^\sigma &= \varphi^\sigma(\delta a, a) \ , \end{aligned} \tag{5-232}$$

$$da^\sigma = \overline{\mu}_\rho^\sigma(a)\delta a^\rho \ , \quad \overline{\mu}_\rho^\sigma(a) = \frac{\partial \varphi^\sigma(b,a)}{\partial b^\rho}\Big|_{b=0} \ . \tag{5-233}$$

Therefore the infinitesimal operators of the intrinsic Lie group in group parameter space are the differential operators

$$\overline{X}_\rho(a) = -\overline{\mu}_\rho^\sigma(a)\frac{\partial}{\partial a^\sigma} \ . \tag{5-234}$$

Racah and Eisenhart called $B_\rho(a) = -\overline{X}_\rho(a)$ the infinitesimal operators of the second parameter group, while we use the same name for $\overline{X}_\rho(a)$.

The definition of the intrinsic state $\Phi_0(X)$ is also identical to the case of finite groups, namely

$$\overline{R}(a)\Phi_0(X) = R(a)\Phi_0(X) \ . \tag{5-235}$$

For further discussion, see Chen, Wang & Gao (1983) and Sec. 6.6.

5.16. The CSCO Approach to the Rep Theory of Lie Groups

In Sec. 3.20, the theory of finite group reps was summarized in seven fundamental theorems. These theorems can be generalized to compact Lie groups.

We first prove that the CSCO-I of the Lie group G and the intrinsic Lie group $\overline{G}$ are equal. From (5-221) we need only prove that any invariant of G is also an invariant of $\overline{G}$, and vice versa, that is,

$$I_i(X_\rho) = I_i(\overline{X}_\rho), \quad i = 1, 2, \ldots, l \ , \tag{5-236}$$

where $I_i(X_\rho)$ are the polynomials of the r infinitesimal operators. From (5-227) we have

$$\begin{aligned} R(a)X_\rho X_\sigma \ldots X_\tau R^{-1}(a) &= R(a)X_\rho R^{-1}(a)R(a)X_\sigma R^{-1}(a)\ldots R(a)X_\tau R^{-1}(a) \\ &= \overline{X}_\rho \overline{X}_\sigma \ldots \overline{X}_\tau \ . \end{aligned} \tag{5-237}$$

Therefore

$$R(a)I_i(X_\rho)R^{-1}(a) = I_i(\overline{X}_\rho) \ , \tag{5-238}$$

and (5-236) follows from (5-217a).

Suppose that $G(s_1)$ is a subgroup of G of rank l_1, and its CSCO-I is designated by

$$C(s_1) = \left(I_1^{(s_1)}(X_\sigma)\ldots I_{l_1}^{(s_1)}(X_\sigma)\right) \ , \tag{5-239}$$

where X_σ are the infinitesimal operators of the subgroup $G(s_1)$. Similarly $\overline{G}(s_1)$ is the subgroup of the intrinsic group $\overline{G}$, and its CSCO-I is designated by

$$\overline{C}(s_1) = \left(I_1^{(s_1)}(\overline{X}_\sigma), \ldots, I_{l_1}^{(s_1)}(\overline{X}_\sigma)\right) \ . \tag{5-240}$$

Now $[C(s_1), \overline{C}(s_1)] = 0$, but $C(s_1) \neq \overline{C}(s_1)$. Suppose furthermore that the Lie group G has a group chain $G \supset G(s), G(s) = G(s_1) \supset G(s_2) \supset \ldots$ We still use $C(s)$ to designate the set of operators

$$C(s) = \left(C(s_1), C(s_2), \ldots\right) \ , \tag{5-241a}$$

where $C(s_i)$ are the CSCO-I of $G(s_i)$. For the intrinsic group chain $\overline{G} \supset \overline{G}(s)$, $\overline{G}(s) = \overline{G}(s_1) \supset \overline{G}(s_2) \supset \ldots$, we have

$$\overline{C}(s) = \left(\overline{C}(s_1), \overline{C}(s_2), \ldots\right) . \tag{5-241b}$$

If the set of operators $K = (C, C(s), \overline{C}(s))$ is a complete set of commuting operators in the group–parameter space, then K is called the CSCO–III of the Lie group. The corresponding group chain is called a canonical subgroup chain, and $(C, C(s))$ is called the CSCO–II of the Lie group.

A CSCO in the space of functions of r variables should consist of r operators. Therefore the CSCO–III for a Lie group of order r contains r operators. Among them, the CSCO–I has already provided l operators; therefore the operator set $C(s)$ should contain $\frac{1}{2}(r-l)$ operators, while the CSCO–II contains $\frac{1}{2}(r+l)$ operators.

The above discussion implies we can use generalizations of the meanings of order g, number g_i of elements in the class i, class operator C_i, scalar product, and so on, given by (5-195)–(5-201), to re–express all the formulas for the rep theory of finite groups so they apply to compact Lie groups. In particular, the seven theorems in the summary of Chapter 3 can be reformulated as follows.

Theorem I: In the class space, the eigenoperator $P^{(\nu)}$ of the CSCO–I of a Lie group G is the projection operator onto the irrep (ν) of G,

$$\begin{aligned} CP^{(\nu)} &= \nu P^{(\nu)} , \\ P^{(\nu)} &= \frac{h_\nu}{g} \int \chi^{(\nu)}(\varphi)^* C(\varphi) \rho(\varphi) d\varphi . \end{aligned} \tag{5-242}$$

where $\chi^{(\nu)}(\varphi) = \chi^{(\nu)}(\varphi^1, \varphi^2, \ldots, \varphi^l)$ is the character depending on l class parameters $\varphi^1, \varphi^2, \ldots, \varphi^l$ (see Sec. 5.29). The projection operators still obey the relation

$$P^{(\nu)} P^{(\mu)} = \delta_{\nu\mu} P^{(\nu)} .$$

Theorem II: In the class–parameter space, the eigenfunctions of the CSCO–I of a Lie group G are the complex conjugates of the characters:

$$C\chi^{(\nu)}(\varphi)^* = \nu \chi^{(\nu)}(\varphi)^* . \tag{5-243}$$

The eigenfunctions of the CSCO–I obey the orthonormality and completeness:

$$\begin{aligned} &\int \frac{g(\varphi)}{g} \chi^{(\nu)}(\varphi)^* \chi^{(\nu')}(\varphi) \rho(\varphi) d\varphi = \delta_{\nu\nu'} , \\ &\sum_\nu \frac{g(\varphi)}{g} \chi^{(\nu)}(\varphi)^* \chi^{(\nu)}(\varphi') \rho(\varphi) = \delta(\varphi - \varphi') , \\ &\delta(\varphi - \varphi') = \delta(\varphi^1 - \varphi'^1) \ldots \delta(\varphi^l - \varphi'^l) , \end{aligned} \tag{5-244}$$

which are the two *orthogonality theorems for characters.*

Theorem III, IV and V in Sec. 3.19 do not need any modification, however, the orthogonality of $\psi_m^{(\nu)\kappa}$ on the intrinsic quantum number κ fails (see (3-273) and (6-73)).

Theorem VI: In group space, the eigenoperators of the CSCO–III of a Lie group G are the projection operators $P_{mk}^{(\nu)}$,

$$\begin{aligned} \begin{pmatrix} C \\ C(s) \\ \overline{C}(s) \end{pmatrix} P_{mk}^{(\nu)} &= \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} P_{mk}^{(\nu)} , \\ P_{mk}^{(\nu)} &= \frac{h_\nu}{g} \int D_{mk}^{(\nu)*}(a) R(a) \rho(a) da . \end{aligned} \tag{5-245a}$$

They still satisfy the relations

$$P^{(\nu)}_{mk} P^{(\mu)}_{lj} = \delta_{\nu\mu}\delta_{kl} P^{(\nu)}_{mj} \ , \tag{5-245b}$$

$$(P^{(\nu)}_{mk})^\dagger = P^{(\nu)}_{km} \ . \tag{5-245c}$$

Theorem VII: In group–parameter space, the eigenfunctions of the CSCO–III of a Lie group G are the complex conjugate of the irreducible matrix elements $D^{(\nu)}_{mk}(a)$

$$\begin{pmatrix} C \\ C(s) \\ \overline{C}(s) \end{pmatrix} D^{(\nu)*}_{mk}(a) = \begin{pmatrix} \nu \\ m \\ k \end{pmatrix} D^{(\nu)*}_{mk}(a) \ . \tag{5-246}$$

The eigenfunctions of the CSCO–III obey orthonormality and completeness relations,

$$\begin{aligned} &\frac{h_\nu}{g} \int D^{(\nu)*}_{mk}(a) D^{(\nu')}_{m'k'}(a) \rho(a) da = \delta_{\nu\nu'}\delta_{mm'}\delta_{kk'} \ , \\ &\sum_{\nu mk} \frac{h_\nu}{g} D^{(\nu)*}_{mk}(a) D^{(\nu)}_{mk}(a') \rho(a) = \delta(a - a') \ , \\ &\delta(a - a') = \delta(a^1 - a'^1) \ldots \delta(a^r - a'^r) \ , \end{aligned} \tag{5-247}$$

which are the two the *orthogonality theorems for irreducible matrix elements.*

The decomposition theorem for the regular rep of finite groups also holds for compact Lie groups. If an arbitrary function $f(a)$ (with no symmetry at all) on the group manifold satisfies the square integrability condition, that is if

$$\frac{1}{g} \int |f(a)|^2 \rho(a) da$$

is finite, then the function $f(a)$ forms a basis for the regular rep of the Lie group (Gel'fand 1963). The function $f(a)$ can be expanded in terms of the orthonormal complete set of functions $\psi^{(\nu)k}_m(a)$,

$$\begin{aligned} &\psi^{(\nu)k}_m(a) = \sqrt{\frac{h_\nu}{g}} D^{(\nu)*}_{mk}(a) \ , \\ &f(a) = \sum_{\nu mk} b^{(\nu)}_{mk} \psi^{(\nu)k}_m(a) \ , \quad b^{(\nu)}_{mk} = \int \psi^{(\nu)k}_m(a)^* f(a) \rho(a) da \ . \end{aligned} \tag{5-248}$$

Therefore the regular rep contains all irreps (ν) of the Lie group G, and the number of occurrence of each irrep equals its dimension h_ν.

5.17. Irreducible Tensors of Lie Groups and Intrinsic Lie Groups

The definition of irreducible tensors of Lie groups is the same as that given for finite groups in Sec. 3.17. If a set of h_ν operators transforms under the group G as

$$T'^{(\nu)}_m = R(a) T^{(\nu)}_m R^{-1}(a) = \sum_t D^{(\nu)}_{tm} T^{(\nu)}_t \ , \tag{5-249}$$

then $T^{(\nu)}_m$ is called an *irreducible tensor* of G . Letting $R(a)$ be an infinitesimal element, we obtain an equivalent definition of irreducible tensor from (5-249),

$$[X_\rho, T^{(\nu)}_m] = \sum_t D^{(\nu)}_{tm}(X_\rho) T^{(\nu)}_t \ . \tag{5-250}$$

Note that for $\nu = \nu_0$ (the adjoint rep) the irreducible matrix $D^{(\nu_0)}$ here is not necessarily identical with $\mathcal{D}^{(\nu_0)}$ in Sec. 5.15. $\mathcal{D}^{(\nu_0)}$ is the irreducible matrix determined by the infinitesimal operators X_ρ. $\mathcal{D}^{(\nu_0)}$ is equivalent to $D^{(\nu_0)}$; however, they are generally not the same. For given $D^{(\nu_0)}$, only through a proper linear combination of X_ρ can we combine them into the ν_0 irreducible tensors $T_m^{(\nu_0)}$ which transform as (5-250). From now on, it is assumed that X_ρ have been chosen to be identical with $T_\rho^{(\nu_0)}$. Under this convention, the expressions (5-208)–(5-211), (5-228) and (5-229) remain valid after replacing $\mathcal{D}^{(\nu_0)}$ with $D^{(\nu_0)}$. For example, (5-211) may be rewritten as

$$[X_\rho, X_\tau] = \sum_\sigma D^{(\nu_0)}_{\sigma\tau}(X_\rho) X_\sigma \ . \tag{5-251}$$

It follows from the anti-isomorphism between $\{\overline{X}_\rho\}$ and $\{X_\rho\}$, that we also have

$$[\overline{X}_\rho, \overline{X}_\tau] = -\sum_\sigma D^{(\nu_0)}_{\sigma\tau}(X_\rho) \overline{X}_\sigma \ . \tag{5-252}$$

Comparing (5-251) with (5-252), a natural extension is to define $\{\overline{X}_\rho\}$ to be the ν_0–irreducible tensor $\{\overline{T}_\rho^{(\nu_0)}\}$ of the intrinsic group $\overline{G}$. Therefore a general definition of the ν–irreducible tensor $\overline{T}_k^{(\nu)}$ of the intrinsic group $\overline{G}$ is

$$[\overline{X}_\rho, \overline{T}_k^{(\nu)}] = -\sum_i D^{(\nu)}_{tk}(X_\rho) \overline{T}_t^{(\nu)} \ . \tag{5-253}$$

In analogy with the irreducible tensors of the group G, two irreducible tensors $\overline{T}_{m_1}^{(\nu_1)}$ and $\overline{T}_{m_2}^{(\nu_2)}$ of $\overline{G}$ can be combined into a third irreducible tensor of $\overline{G}$ using CG coefficients of the group G:

$$\overline{T}_m^{(\nu)\theta} = \sum_{m_1 m_2} C^{(\nu)\theta, m}_{\nu_1 m_1, \nu_2 m_2} \overline{T}^{(\nu_1)}_{m_1} \overline{T}^{(\nu_2)}_{m_2} \ .$$

Let us now prove that the irreducible matrix elements $D^{(\nu)*}_{mk}(a)$ and $D^{(\nu)}_{mk}(a)$ are the irreducible tensors of the groups G and $\overline{G}$, respectively, that is,

$$D^{(\nu)*}_{mk}(a) = T^{(\nu)}_m \ , \quad D^{(\nu)}_{mk}(a) = \overline{T}^{(\nu)}_k \ . \tag{5-254}$$

Regarding $D^{(\nu)}_{mk}(a)$ as a function $u(a)$ on the group manifold and using (5-173) and (5-174), we get

$$\begin{aligned}(1 - \delta a^\rho X_\rho) D^{(\nu)}_{mk}(a) &= D^{(\nu)}_{mk}\big((1 + \delta a^\rho X_\rho) R(a)\big) \\ &= D^{(\nu)}_{mk}\big(R(a)\big) + \delta a^\rho \sum_t D^{(\nu)}_{mt}(X_\rho) D^{(\nu)}_{tk}\big(R(a)\big) \ .\end{aligned}$$

Thus

$$X_\rho D^{(\nu)}_{mk}(a) = -\sum_t \langle \nu m | X_\rho | \nu t \rangle D^{(\nu)}_{tk}(a) \ , \tag{5-255a}$$

$$\langle \nu m | X_\rho | \nu t \rangle = D^{(\nu)}_{mt}(X_\rho) \ . \tag{5-256}$$

Similarly, from (5-230) and (5-231) we have

$$\overline{X}_\rho D^{(\nu)}_{mk}(a) = -\sum_t \langle \nu t | X_\rho | \nu k \rangle D^{(\nu)}_{mt}(a) \ . \tag{5-255b}$$

If the function $u(R_a)$ in (5-173) and (5-230) is chosen as $\tilde{D}^{-1(\nu)}_{mk}(R_a) = \tilde{D}^{(\nu)}_{mk}(R_a^{-1})$, we have

$$X_\rho \tilde{D}^{-1(\nu)}_{mk}(a) = \sum_t \langle \nu t | X_\rho | \nu m \rangle \tilde{D}^{-1(\nu)}_{tk}(a) \ , \tag{5-257a}$$

$$\overline{X}_\rho \tilde{D}^{-1(\nu)}_{mk}(a) = \sum_t \langle \nu k | X_\rho | \nu t \rangle \tilde{D}^{-1(\nu)}_{mt}(a) \ . \tag{5-257b}$$

If $D^{(\nu)}$ is unitary, the above equations become

$$X_\rho D^{(\nu)*}_{mk}(a) = \sum_t \langle \nu t | X_\rho | \nu m \rangle D^{(\nu)*}_{tk}(a) \ , \tag{5-258a}$$

$$\overline{X}_\rho D^{(\nu)*}_{mk}(a) = \sum_t \langle \nu k | X_\rho | \nu t \rangle D^{(\nu)*}_{mt}(a) \ . \tag{5-258b}$$

If the $D^{(\nu)}_{mk}(a)$ and similar objects are regarded as operators, (5-255) and (5-258) should be rewritten as

$$[X_\rho, D^{(\nu)}_{mk}(a)] = -\sum_t \langle \nu m | X_\rho | \nu t \rangle D^{(\nu)}_{tk}(a) \ , \tag{5-259a}$$

$$[\overline{X}_\rho, D^{(\nu)}_{mk}(a)] = -\sum_t \langle \nu t | X_\rho | \nu k \rangle D^{(\nu)}_{mt}(a) \ . \tag{5-259b}$$

$$[X_\rho, D^{(\nu)*}_{mk}(a)] = \sum_t \langle \nu t | X_\rho | \nu m \rangle D^{(\nu)*}_{tk}(a) \ , \tag{5-260a}$$

$$[\overline{X}_\rho, D^{(\nu)*}_{mk}(a)] = \sum_t \langle \nu k | X_\rho | \nu t \rangle D^{(\nu)*}_{mt}(a) \ . \tag{5-260b}$$

Comparing (5-260a) with (5-250), and (5-259b) with (5-253), we see that (5-254) holds.

By means of the Wigner–Eckart theorem (3-319), we have

$$D^{(\nu)}_{tm}(X_\rho) = \langle \nu t | X_\rho | \nu m \rangle = \sum_\theta \langle \nu \| X \| \nu \rangle^\theta C^{(\nu)\theta,t}_{\nu m, \nu_0 \rho} \ , \tag{5-261}$$

where $\theta = 1, 2, \ldots, (\nu_0 \nu \nu)$ is the multiplicity label. Using (5-261), Eqs. (5-259) and (5-260) can now be recast into the following form:

$$[X_\rho, D^{(\nu)}_{mk}(a)] = -\sum_{\theta,t} \langle \nu \| X \| \nu \rangle^\theta C^{(\nu)\theta,m}_{\nu t, \nu_0 \rho} D^{(\nu)}_{tk}(a) \ , \tag{5-262a}$$

$$[\overline{X}_\rho, D^{(\nu)}_{mk}(a)] = -\sum_{\theta t} \langle \nu \| X \| \nu \rangle^{(\theta)} C^{(\nu)\theta,t}_{\nu k, \nu_0 \rho} D^{(\nu)}_{mt}(a) \ , \tag{5-262b}$$

$$[X_\rho, D^{(\nu)*}_{mk}(a)] = \sum_{\theta t} \langle \nu \| X \| \nu \rangle^{(\theta)} C^{(\nu)\theta,t}_{\nu m, \nu_0 \rho} D^{(\nu)*}_{tk}(a) \ , \tag{5-263a}$$

$$[\overline{X}_\rho, D^{(\nu)*}_{mk}(a)] = \sum_{\theta t} \langle \nu \| X \| \nu \rangle^{(\theta)} C^{(\nu)\theta,k}_{\nu t, \nu_0 \rho} D^{(\nu)*}_{mt}(a) \ . \tag{5-263b}$$

Before ending this section, we give an important relation between the matrix elements X_ρ and $\overline{X}_\rho$. Letting R_a and $\overline{R}_a$ in (3-198) be infinitesimal operators, we obtain the required relation

$$\langle \nu m | X_\rho | \nu k \rangle = \langle \nu k | \overline{X}_\rho | \nu m \rangle \ . \tag{5-264}$$

5.18. The Cartan–Weyl Basis

Let A be an arbitrary element of a semi-simple Lie algebra,

$$A = a^\mu X_\mu \ . \tag{5-265}$$

We seek the eigenvector of the operator $\overset{\circ}{A}$,

$$\overset{\circ}{A} X = aX \ , \tag{5-266a}$$

that is, a vector X such that

$$[A, X] = aX \ . \tag{5-266b}$$

Theorem 5.8: If A has the maximum number of distinct eigenvalues, then only the eigenvalue zero is degenerate.

The degeneracy l of the eigenvalue zero is called the *rank* of the Lie algebra. Denoting the l independent eigenvectors associated with the eigenvalue zero by $H_i, i = 1, 2, \ldots, l$, we have

$$[A, H_i] = 0 \ . \tag{5-267}$$

Since $[A, A] = 0$, A is necessarily of the form $A = \lambda^i H_i$. We can choose A as one of the operators H_i, say, $A = H_1$. Using Jacobi's identity (5-45a), we can show that $H_1, \ldots H_l$ form a subalgebra, called the *Cartan subalgebra.* It can be further shown that it is an Abelian subalgebra,

$$[H_i, H_j] = 0 \ . \tag{5-268a}$$

The remaining $r - l$ non–degenerate eigenvectors are denoted by E_α,

$$[H_1, E_\alpha] = \alpha_1 E_\alpha \ . \tag{5-268b}$$

Applying the Jacobi identity to H_1, H_i, E_α and using (5-268), we get

$$\begin{aligned} [H_1, [H_i, E_\alpha]] &= [H_i, [H_1, E_\alpha]] + [[H_1, H_i], E_\alpha] \\ &= \alpha_1 [H_i, E_\alpha] \ . \end{aligned}$$

Since α_1 is non–degenerate, $[H_i, E_\alpha]$ must be proportional to E_α,

$$[H_i, E_\alpha] = \alpha_i E_\alpha \ . \tag{5-268c}$$

Therefore E_α is a simultaneous eigenvector of $H_1, \ldots H_l$ corresponding to the set of eigenvalues $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_l)$. One can regard α as a vector in an l–dimensional space and is called *root vector*, or simply the *root.*

Applying the Jacobi identity once again, we find

$$\begin{aligned} [H_1, [E_\alpha, E_\beta]] &= [E_\alpha, [H_1, E_\beta]] + [[H_1, E_\alpha], E_\beta] \\ &= (\alpha_1 + \beta_1)[E_\alpha, E_\beta] \ . \end{aligned} \tag{5-269a}$$

This shows that $[E_\alpha, E_\beta]$ is an eigenvector of H_1 associated with the root $\alpha + \beta$, if $\alpha + \beta$ is a non–vanishing root, that is,

$$[E_\alpha, E_\beta] = N_{\alpha\beta} E_{\alpha+\beta} \ , \tag{5-269b}$$

where $N_{\alpha\beta}$ is a non–zero normalizing coefficient. If $\beta = -\alpha$, then $[E_\alpha, E_\beta]$ is a linear combination of the H_i, that is,

$$[E_\alpha, E_{-\alpha}] = C^i_{\alpha-\alpha} H_i \ . \tag{5-269c}$$

We thus have

Theorem 5.9: If α is a non–vanishing root of a semi–simple Lie algebra, then $-\alpha$ is also a root.

By choosing the scale (normalization) of the E_α appropriately we can have

$$C^i_{\alpha-\alpha} = \alpha_i \ ,$$

and the commutation relations for a semi–simple Lie algebra can be written in the following form

$$\begin{aligned} &[H_i, H_k] = 0 \ , && [H_i, E_\alpha] = \alpha_i E_\alpha \ , \\ &[E_\alpha, E_{-\alpha}] = (\alpha, H) \equiv \sum_i \alpha_i H_i \ , && [E_\alpha, E_\beta] = N_{\alpha\beta} E_{\alpha+\beta} \ , \end{aligned} \tag{5-270a}$$

where $N_{\alpha\beta} = 0$ if $\alpha + \beta$ is not a root. The basis for a Lie algebra in the form of (5-270a) is called *Cartan-Weyl basis* .

Using the definition (5-213a), from (5-270a) we can calculate the metric tensor $g_{\rho\sigma}$. Following Racah (1951) we use $i, j, k, \ldots = 1, 2, \ldots, l$ for the coordinates in the subspace of dimension l spanned by H_i, while α, β, γ will be used for the $r - l$ dimensional subspace spanned by $E_\alpha, E_\beta, \ldots$. The indices ρ, σ, τ will be used to refer to the whole r–dimensional space. Symbolically,

$$\rho, \sigma, \tau = \big((i, j, k, \ldots); \alpha, \beta, \gamma, \ldots\big) \ .$$

The metric tensor $g_{\alpha\rho}$ can be calculated to be

$$g_{\alpha\rho} = \sum_i \left(C^\alpha_{\alpha i} C^i_{\rho\alpha} + C^i_{\alpha-\alpha} C^{-\alpha}_{\rho i}\right) + \sum_{\beta\neq\alpha} C^{\alpha+\beta}_{\alpha\beta} C^\beta_{\rho,\alpha+\beta} \ . \tag{5-270b}$$

Since $C^i_{\rho\alpha}, C^{-\alpha}_{\rho i}$, and $C^\beta_{\rho,\alpha+\beta}$ vanish unless $\rho = -\alpha$, the $r \times r$ matrix is block diagonal,

$$(g_{\rho\sigma}) = \left(\begin{array}{c|c} (g_{ik}) & \\ \hline & (g_{\alpha\beta}) \end{array}\right) \ .$$

From (5-270a) and (5-270b) we find that

$$g_{\alpha\beta} = \delta_{\alpha+\beta} g_{\alpha-\alpha} \ , \quad g_{\alpha-\alpha} = 2\sum_i \alpha_i \alpha_i + \sum_{\beta\neq\alpha} N_{\alpha\beta} N_{-\alpha,\alpha+\beta} \ .$$

From (5-213a) and (5-268c),

$$g_{ij} = \sum_\alpha C^\alpha_{i\alpha} C^\alpha_{j\alpha} = \sum_\alpha \alpha_i \alpha_j \ . \tag{5-270c}$$

We now define two kinds of *scalar products* for the two roots α and β,

$$\langle \alpha, \beta \rangle = \alpha_i g^{ij} \beta_j = \alpha^i \beta_i \ , \tag{5-270d}$$

$$(\alpha, \beta) = \sum_{i=1}^{l} \alpha_i \beta_i \ . \tag{5-270e}$$

The scalar product $\langle \alpha, \beta \rangle$ is in covariant form, and its value is independent of the normalizations of the generators, while the scalar product (α, β) is scale dependent. The former is more elegant, but the latter is more convenient and familiar to us, since it does not involve the metric tensor g_{ij}. When (g_{ij}) is a unit matrix, $\langle \alpha, \beta \rangle = (\alpha, \beta)$.

By a further choice of the scales of H_i and E_α, we can make the metric tensor takes the following form

$$g_{ij} = \delta_{ij} \ , \quad g_{\alpha\beta} = \delta_{\alpha+\beta} \ , \quad (g_{\rho\sigma}) = (g^{\rho\sigma}) \ . \tag{5-271a}$$

With this choice, there is no distinction between the covariant and contravariant, $\alpha_i = \alpha^i$, and (5-270a) goes over to

$$\begin{aligned} &[H_i, H_k] = 0 \ , && [\mathbf{H}, E_\alpha] = \boldsymbol{\alpha} E_\alpha \ , \\ &[E_\alpha, E_{-\alpha}] = \langle \alpha, H \rangle \ , && [E_\alpha, E_\beta] = N_{\alpha\beta} E_{\alpha+\beta} \ , \\ &\mathbf{H} = (H_1, \ldots, H_l) \ , && \boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_l) \ , \qquad \langle \alpha, H \rangle = \alpha^i H_i \ . \end{aligned} \tag{5-271b}$$

The commutation relation for a semi-simple Lie algebra in the form of (5-271b) is said to be in *standard form*, and its basis is referred to as the *Cartan–Weyl standard basis*, or *standard basis*

for short. Although (5-271b) is more elegant, the generators in (5-270a) and (5-271b) differ only in a multiplicative factor. The former is more often used and is *preferable* because it avoids the tedious calculations of the metric tensor $g_{\rho\sigma}$.

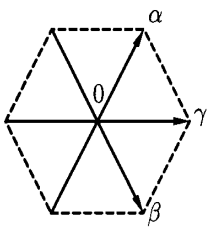
It is to be noted that the difference between the Cartan–Weyl basis and the standard basis lies in the definition of the scalar product,

$$[E_\alpha, E_{-\alpha}] = \begin{cases} (\alpha, H)\ , & \text{for Cartan–Weyl basis} \\ \langle \alpha, H\rangle\ , & \text{for Cartan–Weyl standard basis} \end{cases} \tag{5-271c}$$

Example: The group SU_3. After renormalizing the infinitesimal operators of SU_3 given in (5-160) and with $\alpha = 1, -1, 0$ indexed as $1, 2, 3$ we have

$$\begin{aligned} &H_1 = \tfrac{1}{2\sqrt{3}}(\hat{n}_1 - \hat{n}_2)\ , \quad H_2 = \tfrac{1}{6}(\hat{n}_1 + \hat{n}_2 - 2\hat{n}_3)\ , \\ &E_\alpha = \tfrac{1}{\sqrt{6}} C_1^\dagger C_3\ , \qquad E_\beta = \tfrac{1}{\sqrt{6}} C_3^\dagger C_2\ , \qquad E_\gamma = \tfrac{1}{\sqrt{6}} C_1^\dagger C_2\ , \\ &E_{-\alpha} = \tfrac{1}{\sqrt{6}} C_3^\dagger C_1\ , \qquad E_{-\beta} = \tfrac{1}{\sqrt{6}} C_2^\dagger C_3\ , \qquad E_{-\gamma} = \tfrac{1}{\sqrt{6}} C_2^\dagger C_1\ , \end{aligned} \tag{5-272a}$$

where $\hat{n}_i = C_i^\dagger C_i$. Since $[\hat{n}_i, C_i^\dagger] = C_i^\dagger$ and $[\hat{n}_i, C_i] = -C_i$, we can easily obtain the standard commutators for SU_3 in the form (5-271b) with $N_{\alpha\beta} = \frac{1}{\sqrt{6}}$ if $\alpha + \beta$ is a root and the root vectors are those shown in Fig. 5.18. Such a diagram is called a *root diagram.*



$$\begin{aligned} &\alpha = \tfrac{1}{\sqrt{3}}\left(\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}\right)\ , \\ &\gamma = \tfrac{1}{\sqrt{3}}(1, 0)\ , \quad \langle \alpha, \alpha\rangle = \langle \beta, \beta\rangle = \langle \gamma, \gamma\rangle = \tfrac{1}{3} \\ &\beta = \tfrac{1}{\sqrt{3}}\left(\tfrac{1}{2}, -\tfrac{\sqrt{3}}{2}\right)\ . \end{aligned} \tag{5-272b}$$

Fig. 5.18. The root diagram of SU_3.

It can be shown that the metric tensor for (5-272a) is

$$(g_{\rho\sigma}) = (g^{\rho\sigma}) = \mathbf{g} = \left(\begin{array}{c|cc} \mathbf{I} & & \\ \hline & \mathbf{K} & \\ & & \mathbf{K} \\ & & & \mathbf{K} \end{array}\right), \qquad \mathbf{K} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{5-272c}$$

where $\mathbf{I}$ is a 2×2 unit matrix.

If all the SU_3 generators in (5-272a) are multiplied by a factor of $\sqrt{6}$, i. e. going back to the generators in (5-160), we get the Cartan–Weyl basis of SU_3 which obey (5-270a), and the metric tensor is

$$(g'_{\rho\sigma}) = 6\mathbf{g}, \quad (g'^{\rho\sigma}) = \frac{1}{6}\mathbf{g}\ . \tag{5-272d}$$

Ex. 5.3. To verify the metric tensor of (5-272c).

Ex. 5.4. For the Lie algebras so_5 and so_4, we have $H_1 = \frac{1}{\sqrt{6}}(n_1 - n_{-1}), H_2 = \frac{1}{\sqrt{6}}(n_2 - n_{-2})$, $E_\alpha = E_{ik} = \frac{1}{\sqrt{6}}(C_i^\dagger C_{-k} - C_k^\dagger C_{-i})$, for $i \neq -k$. Show that (i)

$$[\mathbf{H}, E_\alpha] = \boldsymbol{\alpha} E_\alpha\ , \quad [E_\alpha, E_{-\alpha}] = -\boldsymbol{\alpha}\cdot\mathbf{H}\ , \quad \boldsymbol{\alpha} = \tfrac{1}{\sqrt{6}}(\mathbf{e}_i + \mathbf{e}_k)\ ,$$

with $\mathbf{e}_{-i} = -\mathbf{e}_i$ and $\mathbf{e}_0 = 0$, (ii) that the so_5 and so_4 Lie algebras are associated with

the Lie algebras B_2 and D_2, respectively, and (iii) find the metric tensors $(g_{\rho\sigma})$.

5.19. Theorems on Roots

In the following we use the usual definition (5-270e) for the scalar product,

$$(\alpha,\beta) = \sum_i \alpha_i\beta_i = |\alpha||\beta|\cos\theta_{\alpha\beta} \ .$$

Theorem 5.10: If α and β are roots, then $n = 2(\alpha,\beta)/(\alpha,\alpha)$ is an integer and $\beta - \frac{2\alpha(\alpha,\beta)}{(\alpha,\alpha)}$ is also a root.

If $n > 0$, then since

$$[E_\alpha, E_{\beta-n\alpha}] = N_{\alpha,\beta-n\alpha}E_{\beta-(n-1)\alpha} \ ,$$

we know that $\beta - (n-1)\alpha$ is also a root. Thus we have a string of roots,

$$\beta, \beta-\alpha, \ \beta-2\alpha, \ldots, \beta-n\alpha \ ,$$

called the β–string containing α.

Analogously, if $n < 0$, then we have a string of roots

$$\beta, \beta+\alpha, \ \beta+2\alpha, \ldots, \beta+|n|\alpha \ .$$

Theorem 5.11: If α is a root, then $m\alpha$ is not a root for integer $|m| > 1$.

Proof: $[E_\alpha, E_\alpha] = 0$. From (5-269b) 2α is therefore not a root. If $n\alpha$, n an integer greater than 2, were a root, then we would have the string of roots $\alpha, 2\alpha, \ldots n\alpha$, and so that 2α would be a root. But this is a contradiction so $n\alpha$ cannot be a root. A similar argument applies for negative integers. **QED**

Theorem 5.12: If α and β are two roots, then the only possible values of $\frac{2(\alpha,\beta)}{(\alpha,\alpha)}$ are

$$m = \frac{2(\alpha,\beta)}{(\alpha,\alpha)} = 0, \pm1, \pm2, \pm3 \ . \tag{5-273}$$

Therefore, the β–string containing α has at most four roots.

Proof: Suppose that we have a string of five roots $\beta, \beta-\alpha, \ldots, \beta-4\alpha$, which could be a substring of a larger string of roots. By relabelling the roots, they can be written as $\beta-2\alpha, \beta-\alpha, \beta, \beta+\alpha, \beta+2\alpha$.

Since $(\beta+2\alpha) \mp \beta = \begin{cases} 2\alpha \\ 2(\beta+\alpha) \end{cases}$ are not roots, from Theorem 5.10, it follows that

$$(\beta+2\alpha, \beta) = 0 \ . \tag{5-274a}$$

Similarly, since $(\beta-2\alpha) \mp \beta = \begin{cases} -2\alpha \\ 2(\beta-\alpha) \end{cases}$ are not roots, we have

$$(\beta-2\alpha, \beta) = 0 \ . \tag{5-274b}$$

Adding (5-274a) and (5-274b) leads to $(\beta,\beta) = 0$, which implies that $\beta = 0$. Thus we can not have a string consisting of five roots. **QED**

5.20. Root Diagrams

In a space of dimension l, we can "draw" a diagram, called a *root diagram*. Each simple Lie algebra is uniquely associated with a root diagram. The null vector will correspond to H_i. A root diagram carries the following important messages: If in the diagram we have three weights α, β and γ, satisfying $\alpha + \beta = \gamma$, then $[E_\alpha, E_\beta]$ is equal to E_γ to within a multiplicative factor, and if $\alpha + \beta$ is not a root, then E_α and E_β commute.

Equation (5-273) in Theorem 5.12 stipulates the angles and lengths of roots. Let $\theta_{\alpha\beta}$ be the angle between the root vectors α and β. We have

$$\cos\theta_{\alpha\beta} = \frac{(\alpha,\beta)}{\sqrt{(\alpha,\alpha)(\beta,\beta)}} = \frac{\sqrt{mn}}{2}\,, \tag{5-275a}$$

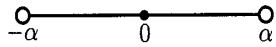
where

$$m = \frac{2(\alpha,\beta)}{(\alpha,\alpha)}, \quad n = \frac{2(\alpha,\beta)}{(\beta,\beta)}\,. \tag{5-275b}$$

It suffices to consider the case with $\cos\theta_{\alpha\beta} > 0 (\theta_{\alpha\beta} < 90)$, since if $(\alpha,\beta) < 0$, then $(-\alpha,\beta) > 0$. From Eq. (5-273), the only possible values of $\theta_{\alpha\beta}$ are as follows:

m	n	$\cos\theta_{\alpha\beta}$	$\theta_{\alpha\beta}$	$\lvert\alpha\rvert^2/\lvert\beta\rvert^2$
1	1	1/2	60°	1
1	2	$\sqrt{2}/2$	45°	2
1	3	$\sqrt{3}/2$	30°	3
2	2	1	0°	1
1	0	0	90°	0
0	0	0	90°	indefinite

Example: For $l = 1$, there are only two non–zero roots, $\pm\alpha$, corresponding to the diagram



For $l = 2$, we have the following diagram. (i) $\theta_{\alpha\beta} = 60°$. The root diagram is a hexagon, as shown in Fig. 5.20-1. There are eight root vectors (including two null roots), corresponding to the Lie algebra su_3. (ii) $\theta_{\alpha\beta} = 45°$. Two diagrams arise, namely, Figs. 5.20-2 and 5.20-3. The former corresponds to the Lie algebra B_2. There are 10 root vectors (including two null vectors), which we may associate with the roots of the so_5 Lie algebra (for the proof, see Ex. 5.3). The latter diagram corresponds to the Lie algebra C_2, which is isomorphic to B_2, since their root diagrams differ only by a rotation through 45°. The Lie algebra C_2 is associated with the roots of the sp_4 Lie algebra (see Ex. 5.4).

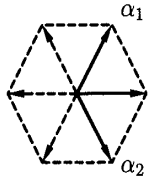


Fig. 5.20-1. Root diagram for A_2.

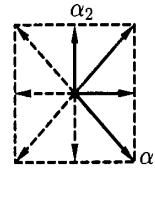


Fig. 5.20-2. Root diagram for B_2.

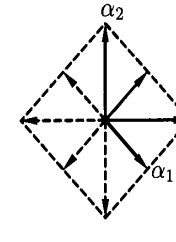


Fig. 5.20-3. Root diagram for C_2.

(iii) $\theta_{\alpha\beta} = 90°$. The diagram is shown in Fig. 5.20-4 and is the root diagram of D_2, which we may associate with the so_4 Lie algebra (see Ex. 5.3). It can be decomposed into two sets of mutually orthogonal roots. According to Theorem 5.1, the root diagram for a semi–simple non–simple group can be decomposed into two orthogonal subdiagrams, each corresponding to a simple group. Here we have $D_2 = A_1 \oplus A_1$, indicating that the Lie algebra of so_4 is isomorphic to $so_3 \oplus so_3$.

Finally $\theta_{\alpha\beta} = 30°$. The diagram is shown in Fig. 5.20-5 which is the root diagram of the exceptional Lie algebra G_2. There are 12 non–zero roots and two null roots.

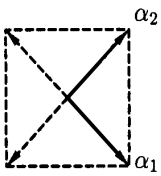


Fig. 5.20-4. Root diagram for D_2.

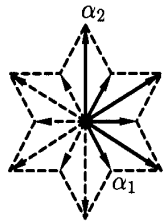


Fig. 5.20-5. Root diagram for G_2.

For Lie algebras A_{l-1}, B_l, C_l and D_l with rank greater than 2, which correspond to the four classical Lie groups SU_l, SO_{2l+1}, Sp_{2l} and SO_{2l}, respectively, the non null root vectors and the positive root set Σ^+ (see Sec. 5.21) can be expressed in terms of the mutually orthogonal unit vectors

$$\mathbf{e}_1 = (1,0,\ldots,0), \quad \mathbf{e}_2 = (0,1,0,\ldots,0),\ldots, \quad \mathbf{e}_l = (0,\ldots 0,1)\ .$$

The generators of A_{l-1}, B_l, C_l and D_l are given in (5-124) (or (5-160)), (5-170), and (5-147). They fulfill (5-270a) and thus are in Cartan–Weyl basis. The corresponding root vectors are given below along with the generators.

1. A_{l-1} $[r = l^2 - 1]$

$$\begin{aligned} &\text{Cartan subalgebra: } H_i = n_i - \tfrac{n}{l}\ , \\ &\text{Root vectors:} \qquad \mathbf{e}_i - \mathbf{e}_j, \quad i \neq j = 1,2,\ldots,l\ , \\ &E_{\alpha^+} : \{C_i^\dagger C_j\}\ , \\ &\Sigma^+ \ : \{\mathbf{e}_i - \mathbf{e}_j\}_1^l, \quad i < j\ . \end{aligned} \tag{5-276a}$$

2. B_l $[r = l(2l+1)]$

$$\begin{aligned} &\text{Cartan subalgebra: } H_i = n_i - n_{-i}\ , \\ &\text{Root vectors:} \qquad \pm\mathbf{e}_i, \ \pm\mathbf{e}_i \pm \mathbf{e}_j, \quad i \neq j = 1,2,\ldots,l\ , \\ &E_{\alpha^+} : \{X_{i0}, X_{i\mp j}\}\ , \\ &\Sigma^+ \ : \{\mathbf{e}_i, \mathbf{e}_i \pm \mathbf{e}_j\}_1^l, \quad i < j\ . \end{aligned} \tag{5-276b}$$

3. C_l $[r = l(2l+1)]$

$$\begin{aligned} &\text{Cartan subalgebra: } H_i = n_i - n_{-i}\ , \\ &\text{Root vectors:} \qquad 2\mathbf{e}_i, \pm\mathbf{e}_i + \mathbf{e}_j, \quad i \neq j = 1,2,\ldots,l\ , \\ &E_{\alpha^+} : \{\sqrt{2}C_i^\dagger C_{-i}, X'_{i\mp j}\}\ , \\ &\Sigma^+ \ : \{2\mathbf{e}_i,\ \mathbf{e}_i \pm \mathbf{e}_j\}_1^l, \quad i < j\ . \end{aligned} \tag{5-276c}$$

4. D_l $[r = l(2l-1)]$

$$\text{Cartan subalgebra: } H_i = n_i - n_{-i}\ ,$$

$$\begin{aligned} &\text{Root vectors:} \qquad \pm\mathbf{e}_i \pm \mathbf{e}_j \quad i \neq j = 1,2,\ldots,l\ , \\ &E_{\alpha^+} : \{X_{i\mp j}\}\ , \\ &\Sigma^+ \ : \{\mathbf{e}_i \pm \mathbf{e}_j\}_1^l, \quad i < j\ , \end{aligned} \tag{5-276d}$$

where

$$X_{ij} = C_i^\dagger C_j - (-1)^{i-j} C_{-j}^\dagger C_{-i}\ , \tag{5-276e}$$

$$X'_{ij} = \delta_i C_i^\dagger C_j - \delta_j C_{-j}^\dagger C_{-i},\ \delta_i = \text{sign}(i)\ . \tag{5-276f}$$

Notice that the $E_{\alpha+}$ of D_l is obtained from that of B_l by ignoring the generators X_{i0}.

Ex. 5.5. Show that the bases in (5-276) fulfill the Cartan–Weyl basis conditions (5-270a).

5.21. The Dynkin Diagram and the Simple Root Representation

Dynkin invented an ingenious scheme to draw the root diagrams for the Lie algebras of any rank. The key point is to focus our attention on the linearly independent root vectors, called the *simple roots*. The two-dimensional diagram for the simple roots, called the *Dynkin diagram*, contains all the necessary information about the root vectors.

A root vector α^+ is called a *positive root* if in some given basis the first non-vanishing component of α^+ is positive. The positive root set is designated Σ^+. For example, the solid lines in Fig. 5.20 represent the positive roots for the ordinary Cartesian basis.

A positive root is said to be *simple* if it cannot be decomposed into the sum of two positive roots. For example, the solid lines labelled α_i in Fig. 5.20 represent the simple roots.

For a semi-simple Lie algebra of rank l, there are l simple roots, denoted by $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \ldots, \boldsymbol{\alpha}_l$, which form a basis for the l-dimensional *root space* . The metric tensor is

$$g_{ij} = (\boldsymbol{\alpha}_i, \boldsymbol{\alpha}_j)\ . \tag{5-277a}$$

It is important not to confuse the metric tensor g_{ij} in the root space spanned by the l simple roots $\boldsymbol{\alpha}_i$ with the metric tensor $g_{ij} = \langle H_i, H_j \rangle$ of (5-270c) in the space spanned by H_i. For example, for the SU_3 Lie algebra (5-272a),

$$(g_{ij}) = \frac{1}{6}\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}, \qquad (g_{ij}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\ . \tag{5-277b}$$

Theorem 5.13: If α and β are two simple roots, then $\alpha - \beta$ is not a root.

Proof: Suppose that $\alpha - \beta = \gamma$ were a positive root, then $\alpha = \beta + \gamma$, violating the hypothesis that α is a simple root. Suppose that $\alpha - \beta = \gamma$ were a negative root, then $\alpha = \beta + (-\gamma)$, again violating the hypothesis that α is a simple root. Hence $\alpha - \beta$ cannot be a root. **QED**

Theorem 5.14: If α and β are two simple roots, then $\theta_{\alpha\beta}$ can only equal $90°, 120°, 135°$, or $150°$.

If $|\alpha| < |\beta|$, then we have the table in Fig. 5.21-1, where we associate the simple roots α and β with circles joined by one, two, or three lines for $(|\beta|/|\alpha|)^2 = 1, 2, 3$, respectively, or left unjoined for $\theta_{\alpha\beta} = 90°$. Circles corresponding to the shorter roots are filled, while those to the longer roots are left open (for any semi-simple Lie algebra, there exist simple roots of at most two distinct lengths).

These are the prototypes for the *Dynkin diagrams* (they are the Dynkin diagrams for $A_2, B_2 \approx C_2, G_2$ and D_2, respectively). The Dynkin diagrams and simple roots for A_l, B_l, C_l, and D_l are shown in Fig. 5.21-2. From Fig. 5.21-2 the following isomorphism is readily seen: $A_1 \approx B_1 \approx C_1, B_2 \approx C_2, D_2 \approx A_1 \oplus A_1, A_3 \approx D_3$.

θ	$\cos\theta_{\alpha\beta}$	$\lvert\beta\rvert^2/\lvert\alpha\rvert^2$		Dynkin diagram	$\frac{2(\alpha,\beta)}{(\alpha,\alpha)}$	$\frac{2(\alpha,\beta)}{(\beta,\beta)}$
120°	$-1/2$	1	A_2		-1	-1
135°	$-\sqrt{2}/2$	2	$B_2(C_2)$		-2	-1
150°	$-\sqrt{3}/2$	3	G_2		-3	-1
90°	0		D_2		0	0

Fig. 5.21-1. Simple roots and related variables.

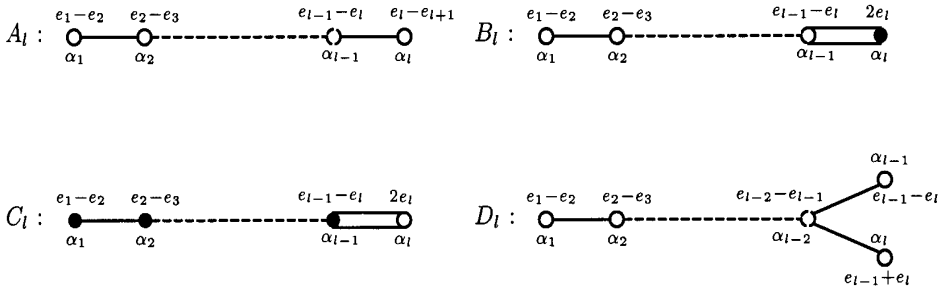


Fig. 5.21-2. The Dynkin diagrams and simple roots of A_l, B_l, C_l and D_l.

Apart from these four infinite series of diagrams, there are only five other possible diagrams, which corresponds to the exceptional Lie algebra G_2, F_4, E_6, E_7, and E_8. All the Dynkin diagrams shown in Figs. 5.21-2 and 5.21-3.

Any root vector $\mathbf{v}$ can be expressed as

$$\mathbf{v} = \sum_{i=1}^{l} v^i_{SRS} \boldsymbol{\alpha}_i \ , \tag{5-278a}$$

and

$$\{\mathbf{v}\}_{SRS} \equiv \{v^1, v^2, \ldots, v^l\}_{SRS} \tag{5-278b}$$

is referred to as the representative of the root vector $\mathbf{v}$ in the *simple roots representation* (SRS) (in the sense used in quantum mechanics), or simply the SRS representative of $\mathbf{v}$. The curly brackets are reserved for the SRS representatives.

The basis $\{\boldsymbol{\alpha}_i\}$ is not an orthonormal one. We may introduce the dual basis $\{\bar{\boldsymbol{\alpha}}^i\}$ such that

$$(\bar{\boldsymbol{\alpha}}^j, \boldsymbol{\alpha}_i) = \delta_{ij}, \quad \sum_{i=1}^{l} |\boldsymbol{\alpha}_i)(\bar{\boldsymbol{\alpha}}^i| = 1 \ . \tag{5-279}$$

Therefore

$$v^i_{SRS} = (\bar{\boldsymbol{\alpha}}^i, \mathbf{v}) \ . \tag{5-280}$$

If $\boldsymbol{\beta}$ is a positive root, then its SRS coordinates $(\bar{\boldsymbol{\alpha}}^i, \boldsymbol{\beta})$ are all non-negative. The set of l simple roots is designated Π.

5.22. The Cartan Matrix

The *Cartan matrix* for a given Lie algebra with the simple roots $\alpha_1, \alpha_2, \ldots, \alpha_l$ is defined by

$$A_{ij} = \frac{2(\alpha_i, \alpha_j)}{(\alpha_i, \alpha_i)} = \frac{g_{ij}}{N_i} \ , \quad N_i \equiv \frac{(\alpha_i, \alpha_i)}{2} \ . \tag{5-281a}$$

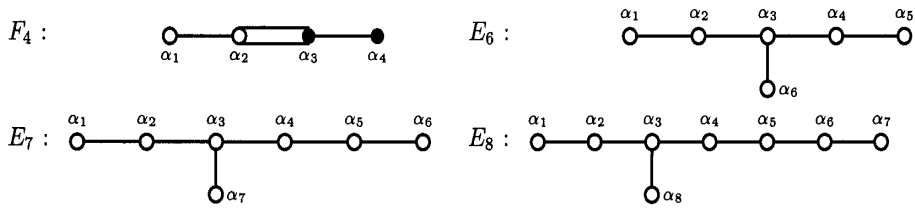


Fig. 5.21-3. The Dynkin diagrams of the four exceptional Lie algebras, F_4, E_6, E_7 and E_8.

The diagonal matrix elements of A are always equal to 2, while the off diagonal matrix elements are restricted to the values 0, $-1, -2$ and -3. Given any Dynkin diagram, using (5-281a), we can readily construct its associated Cartan matrix. For example, for G_2, we have

$$\alpha_1 \Longleftarrow \alpha_2 , \quad A = \begin{array}{c} \begin{matrix} \alpha_1 & \alpha_2 \end{matrix} \\ \begin{pmatrix} 2 & -1 \\ -3 & 2 \end{pmatrix} \end{array} . \tag{5-281b}$$

Similarly for A_l, B_l, C_l and D_l, we have

$$A_l : A = \begin{bmatrix} 2 & -1 & 0 & & & \\ -1 & 2 & -1 & & & \\ 0 & -1 & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & -1 & 0 \\ & & & & -1 & 2 & -1 \\ & & & & 0 & -1 & 2 \end{bmatrix} , \quad B_l : A = \begin{bmatrix} 2 & -1 & 0 & & & \\ -1 & 2 & -1 & & & \\ 0 & -1 & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & -1 & 0 \\ & & & & -1 & 2 & -1 \\ & & & & 0 & -2 & 2 \end{bmatrix} ,$$

(5-282a, b)

$$C_l : A = \begin{bmatrix} 2 & -1 & 0 & & & \\ -1 & 2 & -1 & & & \\ 0 & -1 & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & -1 & 0 \\ & & & & -1 & 2 & -2 \\ & & & & 0 & -1 & 2 \end{bmatrix} , \quad \begin{matrix} D_l : A \\ (l \geq 4) \end{matrix} = \begin{bmatrix} 2 & -1 & 0 & & & \\ -1 & 2 & -1 & & & \\ 0 & -1 & 2 & & & \\ & & & \ddots & & \\ & & & & -1 & 0 & 0 \\ & & & & 2 & -1 & -1 \\ & & & & -1 & 2 & 0 \\ & & & & -1 & 0 & 2 \end{bmatrix} .$$

(5-282c, d)

Ex. 5.6. For the sp_4 Lie algebra, we have $H_1 = n_1 - n_{-1}, H_2 = n_2 - n_{-2}$, $E_{ik} = \delta_i C_i^\dagger C_{-k}$ $+\delta_k C_k^\dagger C_{-i}$, $(ik) = \pm(1,1), \pm(1,2), \pm(1,-2), \pm(2,2)$. Find the commutators of these operators, draw the corresponding root diagram and show that it is the root diagram of C_2.

Ex. 5.7. Construct the Cartan matrices for the exceptional Lie algebras F_4, E_6, E_7 and E_8 with the Dynkin diagrams shown in Fig. 5.21-3.

Ex. 5.8. Prove that the roots shown in Fig. 5.21-2 are simple.

5.23. Theorems on Weights

We pointed out in Sec. 5.16 that the CSCO–II for a Lie group of order r and rank l contains $\frac{1}{2}(r+l)$ operators. Among them are the l operators, $I_1, \ldots, I_l$, from the CSCO–I of G. The

other l operators can be chosen as the elements of the Cartan subalgebra, $H_1, \ldots, H_l$. The irreducible basis of G is an eigenvector of the CSCO–II of G, and can be denoted by

$$\psi_m^{(\nu)} = \psi_{\Lambda_1 \ldots \Lambda_l, \xi}^{(I_1, \ldots I_l)} , \tag{5-283a}$$

where ξ designates the quantum numbers of the $(r-3l)/2$ remaining operators. For brevity, the irreducible basis (5-283a) is simply written as ψ_Λ,

$$H_i \psi_\Lambda = \Lambda_i \psi_\Lambda , \quad \Lambda = (\Lambda_1, \Lambda_2, \ldots, \Lambda_l) . \tag{5-283b}$$

The l–dimensional vector Λ is called the *weight vector*, or *weight* of the eigenket ψ_Λ. Comparing (5-283b) with (5-270a) we see that the roots are the weights of the adjoint representation.

A weight is said to be *positive* if its first non–vanishing component is positive. A weight Λ is said to be higher than Λ', if $\Lambda - \Lambda'$ is positive. If the weight Λ is higher than any weight M in a set of weights, Λ is called the *highest weight*. A weight is said to be *simple* if it has no degeneracy.

Theorem 5.15: Every rep has at least one weight.

Theorem 5.16: Eigenvectors with distinct weights are linearly independent.

Theorem 5.17: If a rep is irreducible, then its highest weight is simple.

Theorem 5.18: Two irreps are equivalent if and only if they have the same highest weight.

Therefore, we can use the highest weight Λ to label an irrep of a Lie group.

Theorem 5.19: If ψ_Λ is a vector of weight Λ, then $E_\beta \psi_\Lambda$ is of weight $\Lambda + \beta$.

Proof: $H_i E_\beta \psi_\Lambda = \big([H_i, E_\beta] + E_\beta H_i\big)\psi_\Lambda = (\beta_i + \Lambda_i) E_\beta \psi_\Lambda$. **QED**

E_β is called the *step operator*, and is a generalization of $J_\pm$.

Let ψ_Λ be the basis vector of an irrep with the highest weight Λ, then according to Theorem 5.19, we have

$$E_\alpha \psi_\Lambda = 0, \quad \text{for positive roots } \alpha . \tag{5-283c}$$

In parallel with Theorem 5.10, we have

Theorem 5.20: Let Λ be one of the weights of an irrep and α be a root; then $n = 2(\Lambda, \alpha)/(\alpha, \alpha)$ is an integer and $\Lambda' = \Lambda - n\alpha$ is a weight of this irrep.

The weight $\Lambda - n\alpha$ is the image of Λ with respect to the hyperplane S_α through the origin and perpendicular to the root α (see Fig. 5.23-1). The finite group generated by the reflections $S_{\alpha_i}, i = 1, 2, \ldots, l$, is called the *Weyl reflection group.*

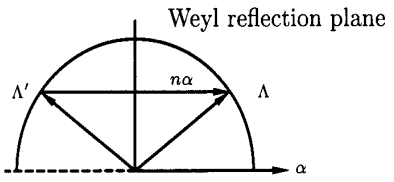


Fig. 5.23-1. The equivalent weights Λ and Λ' are related by a reflection.

Two weights are said to be *equivalent* if we can pass from one to the other by an operation of the Weyl group.

Theorem 5.21: Equivalent weights have the same multiplicity (or degeneracy). In a set of equivalent weights, the highest one is called the *dominant weight.*

Weights of Kronecker products

Let $\Delta(\Lambda)$ be the *complete set of weights* (CSW) for the irrep Λ. Since the eigenvalues of H_i are additive quantum numbers, the CSW of the Kronecker product $(\Lambda \times \Lambda')$ is

$$\Delta(\Lambda \times \Lambda') = \Delta(\Lambda) + \Delta(\Lambda') \ , \tag{5-284a}$$

that is an arithmetic sum where every weight of $\Delta(\Lambda')$ is added to every weight of $\Delta(\Lambda)$. Equation (3-284a) is a generalization of $M = m + m'$ for eigenvalues of J_z.

Suppose that $|1\rangle, |2\rangle, \ldots |n\rangle$ carry the defining rep [1] of a linear transformation group G_n, which could be $GL(n), SU_n, SO_n$ or Sp_n. The weights of the rep [1] are assumed to be $\Lambda_1 > \Lambda_2 > \ldots > \Lambda_n$. The anti-symmetric states

$$\left| \begin{array}{|c|}\hline i_1 \\ \hline i_2 \\ \hline \vdots \\ \hline i_k \\ \hline \end{array} \right\rangle \tag{5-284b}$$

carry a $\binom{n}{k}$–dimensional rep $M^{[1^k]}$ of G_n with the CSW

$$\Lambda_{i_1} + \Lambda_{i_2} + \ldots + \Lambda_{i_k}, \quad i_1 < i_2 < \ldots < i_k \ . \tag{5-284c}$$

The highest weight in $M^{[1^k]}$ is

$$\Lambda = \Lambda_1 + \Lambda_2 + \ldots + \Lambda_k \ , \tag{5-284d}$$

which corresponds to an irrep designated $(M^{[1^k]})_{\text{h.w.}}$.

Analogously, the symmetric states

$$| \boxed{i_1}\boxed{i_2}\cdots\boxed{i_k} \rangle \tag{5-284e}$$

carry the symmetric representation $M^{[k]}$ of G_n. Its dimension can be calculated in the following way. Replace the k integers $i_1, i_2, \cdots, i_k$ in (5-284e) by $i_1, i_2 + 1, \cdots, i_k + k - 1$, respectively. Now all these k integers are distinct, and each i can take values from 1 to n. Therefore the dimension of the rep $M^{[k]}$ of G_n is ,

$$h^{M^{[k]}}(G_n) = \binom{n+k-1}{k}. \tag{5-284f}$$

The CSW of the rep $M^{[k]}$ is

$$\Lambda_{i_1} + \Lambda_{i_2} + \ldots + \Lambda_{i_k}, \quad i_1 \leq i_2 \leq \ldots \leq i_k \ . \tag{5-284g}$$

The highest weight in $M^{[k]}$ is $k\Lambda_1$, corresponding to an irrep designated by $(M^{[k]})_{\text{h.w.}}$.

Notice that the representations $M^{[1^k]}$ and $M^{[k]}$ are irreducible for the groups $GL(n)$ and SU_n, and denoted by $[1^k]$ and $[k]$, respectively.

Example: The SU_3 group.

1. Irrep [1]. The three flavor quarks u, d, and s carry the irrep [1] of SU_3. The Cartan subalgebra consists of

$$H_1 = \frac{1}{2\sqrt{3}}(n_u - n_d) \ , \quad H_2 = \frac{1}{6}(n_u + n_d - 2n_s) \ . \tag{5-285a}$$

The three weights are

$$\begin{aligned}\Lambda_u &= \frac{1}{\sqrt{3}}\Big(\frac{1}{2},\frac{1}{2\sqrt{3}}\Big) = \frac{1}{3}(2\alpha+\beta)\ ,\\ \Lambda_d &= \frac{1}{\sqrt{3}}\Big(-\frac{1}{2},\frac{1}{2\sqrt{3}}\Big) = \frac{1}{3}(-\alpha-2\beta)\\ \Lambda_s &= \frac{1}{\sqrt{3}}\Big(0,-\frac{1}{\sqrt{3}}\Big) = \frac{1}{3}(-\alpha+\beta)\ ,\end{aligned} \tag{5-285b}$$

where $\Lambda_u > \Lambda_s > \Lambda_d$, while α and β are given by (5-272b).

2. Irrep $[1^2]$. The basis vectors are $\tilde{u} = \boxed{\begin{matrix}d\\s\end{matrix}}$, $\tilde{d} = \boxed{\begin{matrix}u\\s\end{matrix}}$, $\tilde{s} = \boxed{\begin{matrix}u\\d\end{matrix}}$ with the weights

$$\Lambda_{\tilde{u}} = -\Lambda_u, \quad \Lambda_{\tilde{d}} = -\Lambda_d, \quad \Lambda_{\tilde{s}} = -\Lambda_s\ . \tag{5-286}$$

3. Irrep [21]. The basis vectors for the irrep [21] are $|\begin{smallmatrix}uu\\d\end{smallmatrix}\rangle$ and so on, (see Sec. 7.5) as shown on the outer perimeter and the origin of Fig. 5.23-2. The weights are just the roots of SU_3. The weights for the SU_3 irreps [1], [11] and [21] are shown in Fig. 5.23-2. Notice that Λ_u, Λ_d, and Λ_s are equivalent weights and that the six weights on the outer perimeter are also equivalent weights.

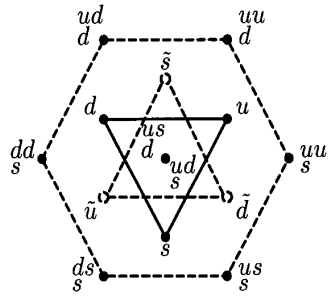


Fig. 5.23-2. The weights for the irreps [1], [11] and [21] of SU_3.

The SU_3 weights can also be expressed in the basis $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$. From Fig. 5.21-2, we have $\alpha = (\mathbf{e}_1 - \mathbf{e}_2)$, $\beta = (\mathbf{e}_2 - \mathbf{e}_3)$. Using (5-285b) we get

$$\Lambda_u = \Big(\frac{2}{3},-\frac{1}{3},-\frac{1}{3}\Big), \quad \Lambda_s = \Big(-\frac{1}{3},\frac{2}{3},-\frac{1}{3}\Big), \quad \Lambda_d = \Big(-\frac{1}{3},-\frac{1}{3},\frac{2}{3}\Big)\ , \tag{5-287a}$$

or

$$\Lambda_i = \mathbf{e}_i - \frac{1}{3}(\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3)\ , \tag{5-287b}$$

where $i = 1, 2$, and 3 refer to u, s and d, respectively. The Λ_i are eigenvalues of the elements of the Cartan subalgebra,

$$H_i = n_i - \frac{1}{3}(n_1+n_2+n_3)\ . \tag{5-287c}$$

5.24. The Dynkin Representation and the Chevalley Basis

5.24.1. The Dynkin representation

With each root vector or weight vector $\mathbf{v}$ we associate a set of numbers

$$(\mathbf{v})^{\mathrm{DYN}} \equiv (v_1,\ldots,v_l)^{\mathrm{DYN}}\ , \tag{5-288a}$$

$$v_i^{\mathrm{DYN}} = 2\frac{(\alpha_i, \mathbf{v})}{(\alpha_i, \alpha_i)} , \tag{5-288b}$$

and call it the representative of $\mathbf{v}$ in the *Dynkin* (DYN) *representation.* Henceforth, the round brackets will be used to denote the DYN representatives. By Theorems 5.10 and 5.20, the coordinates v_i^{DYN} of any root or weight vector $\mathbf{v}$ are integers.

Theorem 5.22: If Λ is the highest weight of a representation (either reducible or irreducible), then its DYN coordinates a_i in $\Lambda = (a_1, a_2, \ldots, a_l)$ are all non-negative.

The DYN representative $(a_1, \ldots a_l)$ of a highest weight is called the *Dynkin label* of the irrep.

Theorem 5.23: If $\mathbf{R}$ is half of the sum of the positive roots,

$$\mathbf{R} = \frac{1}{2}\sum_{\alpha>0} \alpha , \tag{5-288c}$$

then

$$(\mathbf{R})^{\mathrm{DYN}} = (1, 1, \ldots, 1) . \tag{5-288d}$$

For a Lie group of rank l, there are l *basic irreps* with the highest weights denoted by $\mathbf{M}^j, j = 1, 2, \ldots, l$, whose DYN representatives are $(1, 0, \ldots, 0), (0, 1, 0, \ldots, 0), \ldots$ and $(0, \ldots, 0, 1)$, that is.

$$(\mathbf{M}^j)^{\mathrm{DYN}} = (m_1^j, m_2^j, \ldots, m_l^j) , \tag{5-289a}$$

$$m_i^j = 2\frac{(\alpha_i, \mathbf{M}^j)}{(\alpha_i, \alpha_i)} = \delta_{ij} , \quad i, j = 1, 2, \ldots, l . \tag{5-289b}$$

Obviously, $\mathbf{M}^1, \mathbf{M}^2, \ldots, \mathbf{M}^l$ are the basis vectors of the DYN representation, that is,

$$\mathbf{v} = \sum_{i=1}^{l} v_i^{\mathrm{DYN}} \mathbf{M}^i . \tag{5-290a}$$

The weight $\mathbf{M}^i$ will be referred to as the i-th *basic weight.*

As for the SRS in Eq. (5-279), we can introduce a dual basis $\overline{\mathbf{M}}_i$,

$$(\overline{\mathbf{M}}_i, \mathbf{M}^j) = \delta_{ij} , \quad \sum_{i=1}^{l} |\mathbf{M}^i)(\overline{\mathbf{M}}_i| = 1 . \tag{5-291}$$

Thus

$$v_i^{\mathrm{DYN}} = (\overline{\mathbf{M}}_i, \mathbf{v}) . \tag{5-290b}$$

It is easy to see that the two basic weights of SU_3 are $\mathbf{M}^1 = \Lambda_u$ and $\mathbf{M}^2 = \Lambda_{\bar{d}}$ as given in (5-285) and (5-286).

Theorem 5.24: The simple roots α_j and basic weights $\mathbf{M}^j, j = 1, 2, \ldots, l$, form a *bi-orthogonal basis* .

Proof: The proof is trivial, since from (5-289b) we have

$$(\mathbf{M}^j, \alpha_i) = N_i \delta_{ij} , \; N_i = (\alpha_i, \alpha_i)/2 . \tag{5-292}$$

Therefore, $\mathbf{M}^j$ is orthogonal to α_i for $i \neq j$. **QED**

Figure 5.24 illustrates this bi-orthogonality for the Lie algebras of rank two.

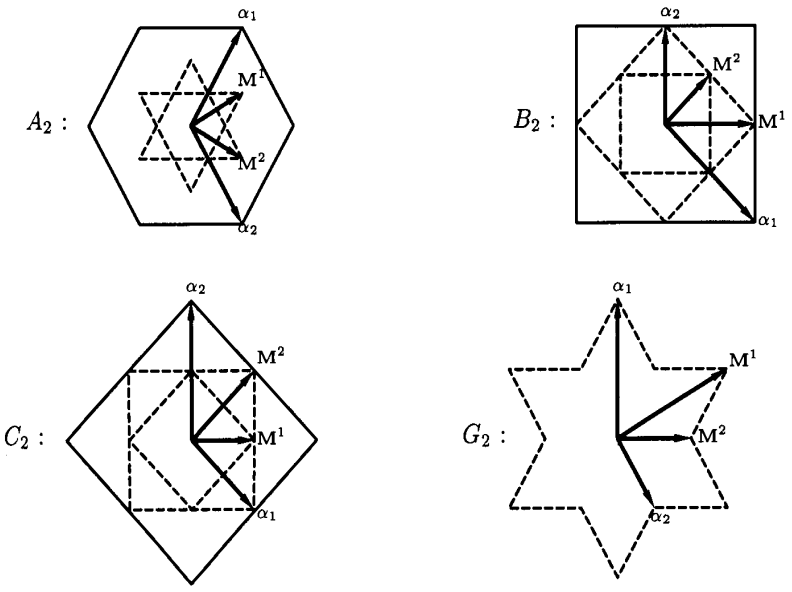


Fig. 5.24. Bi–orthogonal bases formed by simple roots and basic weights.

From (5-292), (5-279), (5-291) and (5-281a) we infer that

$$\overline{\alpha}^{\,i} = N_i^{-1}\mathbf{M}^i \ , \quad \overline{\mathbf{M}}_i = N_i^{-1}\alpha_i \ , \tag{5-293a,b}$$

$$A_{ij} = (\overline{\mathbf{M}}_i, \alpha_j) \ , \tag{5-294a}$$

which in turn means that

$$\alpha_j = \sum_i A_{ij}\mathbf{M}^i \ . \tag{5-294b}$$

Comparing this with (5-290a), we have

$$(\alpha_j)^{\mathrm{DYN}} = (A_{1j}, \ldots, A_{lj}) \ , \tag{5-294c}$$

which shows that the *j–th column of the Cartan matrix A gives the DYN representative of the simple root* α_j.

3. The inverse of (5-294b) is

$$\mathbf{M}^j = \sum_i (A^{-1})_{ij}\alpha_i \ . \tag{5-295a}$$

Therefore we have

$$(A^{-1})_{ij} = (\overline{\alpha}^{\,i}, \mathbf{M}^j) \ , \tag{5-295b}$$

$$\{\mathbf{M}^j\}_{\mathrm{SRS}} = \{(A^{-1})_{1j}, \ldots, (A^{-1})_{lj}\} \ , \tag{5-295c}$$

which shows that the *j–th column of the inverse of the Cartan matrix,* A^{-1}, *gives the SRS representative of the basic weight* $\mathbf{M}^j$.

Equations (5-294c) and (5-295c) can be put into a more explicit form, namely,

$$A = \begin{bmatrix} \alpha_1 & \alpha_2 & & \alpha_l \\ A_{11} & A_{12} & \cdots & A_{1l} \\ A_{21} & A_{22} & \cdots & A_{2l} \\ \vdots & \vdots & \vdots & \vdots \\ A_{l1} & A_{l2} & \cdots & A_{ll} \end{bmatrix} \quad \text{(DYN)} \quad , \qquad A^{-1} = \begin{bmatrix} \mathbf{M}^1 & \mathbf{M}^2 & & \mathbf{M}^l \\ A_{11}^{-1} & A_{12}^{-1} & \cdots & A_{1l}^{-1} \\ A_{21}^{-1} & A_{22}^{-1} & \cdots & A_{2l}^{-1} \\ \vdots & \vdots & \vdots & \vdots \\ A_{l1}^{-1} & A_{l2}^{-1} & \cdots & A_{ll}^{-1} \end{bmatrix} \quad \{\text{SRS}\} \quad , \tag{5-296}$$

where $A_{ij}^{-1} \equiv (A^{-1})_{ij}$. The interpretation of the Cartan matrix and its inverse A^{-1} given in (5-296) is very useful and should be kept well in mind.

From (5-280) and (5-293a) we obtain the counterpart of (5-288b), that is,

$$v_{\text{SRS}}^i = 2\frac{(\mathbf{M}^i, \mathbf{v})}{(\alpha_i, \alpha_i)} \, . \tag{5-297}$$

Since the coordinates and the basis vectors transform contragrediently, we have from (5-295)

$$v_i^{\text{DYN}} = \sum_j A_{ij} v_{\text{SRS}}^j \, . \tag{5-298}$$

Equation (5-298) and its inverse can be written as

$$(\mathbf{v})^{\text{DYN}} = A\{\mathbf{v}\}_{\text{SRS}} \, , \quad \{\mathbf{v}\}_{\text{SRS}} = A^{-1}(\mathbf{v})^{\text{DYN}} \, , \tag{5-299a, b}$$

where $(\mathbf{v})^{\text{DYN}}$ and $\{\mathbf{v}\}_{\text{SRS}}$ are treated as column vectors.

The inverse Cartan matrices associated with the Dynkin diagrams for the Lie algebras A_l, B_l, C_l and D_l given in Fig. 5.21-2 are shown below with $k(i)$ as the row (column) index, and we note that the expression for $A_{D_l}^{-1}$ is for $l \geq 4$.

$$A_{A_l}^{-1} = \frac{1}{l+1} \left[\begin{array}{cccc|cc} & & & & 2 & 1 \\ & & & & 4 & 2 \\ & & & & 6 & 3 \\ & & & & \vdots & \vdots \\ \hline 2 & 4 & 6 & \ldots & 2l-2, & l-1 \\ 1 & 2 & 3 & \ldots & l-1, & l \end{array}\right] \begin{array}{l} i \rightarrow \\ k \downarrow \\ (l+1-i)k \\ (l+1-k)i \end{array} \quad A_l : \quad , \qquad A_{B_l}^{-1} = \frac{1}{2} \left[\begin{array}{cc|cc} & & 2 & 1 \\ & 2k & 4 & 2 \\ & & 6 & 3 \\ & 2i & \vdots & \vdots \\ \hline & & 2l-2, & l-1 \\ & & 2l-2, & l \end{array}\right] \quad B_l : \quad , \tag{5-300a, b}$$

$$A_{C_l}^{-1} = \tilde{A}_{B_l}^{-1} \, , \quad A_{D_l}^{-1} = \frac{1}{4} \left[\begin{array}{cc|cc} & & 2 & 2 \\ & 4k & 4 & 4 \\ & & 6 & 6 \\ & 4i & \vdots & \vdots \\ \hline 2 & 4 & 6 \ldots & l, \quad l-2 \\ 2 & 4 & 6 \ldots & l-2, \quad l \end{array}\right] \quad D_l (l \geq 4) \, . \tag{5-300c, d}$$

For example, for $A_3, A^{-1} = \frac{1}{4}\begin{pmatrix} 3 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 3 \end{pmatrix}$, $\mathbf{M}^1 = \frac{1}{4}(3\alpha_1 + 2\alpha_2 + \alpha_3), \mathbf{M}^2 = \frac{1}{4}(2\alpha_1 + 4\alpha_2 + 2\alpha_3)$ and $\mathbf{M}^3 = \frac{1}{4}(\alpha_1 + 2\alpha_2 + 3\alpha_3)$.

5.24.2. The eigenvalues of the Casimir operators

For computing the dimensions of irreps, or the eigenvalues of the Casimir operators, we often come across scalar products of the form $(\Lambda, \Lambda), (\Lambda, \beta)$ and (α, β). The evaluation of the scalar

product can be carried out either in the DYN or SRS representation, or preferably, for one vector in the DYN representation and the other in the SRS representation. Using (5-277a), (5-290a) and (5-292) we have

$$(\mathbf{u},\mathbf{v}) = (\mathbf{v},\mathbf{u}) = \sum_{ij} u^i_{\mathrm{SRS}}\, g_{ij}\, v^j_{\mathrm{SRS}} = \sum_i u^i_{\mathrm{SRS}}\, v_i^{\mathrm{DYN}}\, N_i \ . \tag{5-301}$$

The *dimension* of an irrep is given by the Weyl formula

$$\dim(\Lambda) = \prod_{\alpha^+\in\Sigma^+} \frac{(\Lambda+R,\alpha^+)}{(R,\alpha^+)} \ . \tag{5-302}$$

The *Casimir operator* (5-220a) is (Wybourne 1974)

$$\mathcal{C} = X_\rho g^{\rho\sigma} X_\sigma = H_i g^{ik} H_k + \sum_\alpha g^{\alpha-\alpha} E_\alpha E_{-\alpha} \ . \tag{5-303a}$$

Suppose that $|\Lambda\rangle$ is the highest weight state, then $E_{\alpha^+}|\Lambda\rangle = 0$. In the standard basis (5-271b), $g^{\alpha-\alpha}$=1 and $[E_\alpha, E_{-\alpha}] = \langle\alpha, H\rangle$. Therefore

$$\begin{aligned}\mathcal{C}|\Lambda\rangle &= \left(\Lambda_i g^{ik}\Lambda_k + \sum_{\alpha>0}[E_\alpha, E_{-\alpha}]\right)|\Lambda\rangle \\ &= \left[\langle\Lambda,\Lambda\rangle + \sum_{\alpha>0}\langle\alpha,\Lambda\rangle\right]|\Lambda\rangle \ .\end{aligned}$$

Hence, the eigenvalue of the Casimir operator is given by

$$\mathcal{C}(\Lambda) = \langle\Lambda, \Lambda+2R\rangle \ . \tag{5-303b}$$

Note that

$$\langle\Lambda,\Lambda'\rangle = \Lambda_i g^{ik}\Lambda'_k = \Lambda^i_{\mathrm{SRS}}\, g_{ik}\, \Lambda'^k_{\mathrm{SRS}} = \tfrac{1}{2}\sum_k \Lambda^k_{\mathrm{SRS}}\, \Lambda'^{\mathrm{DYN}}_k \langle\alpha_k,\alpha_k\rangle \ .$$

Using (5-301) and (5-288d), we have the eigenvalue

$$\mathcal{C}(\Lambda) = \tfrac{1}{2}\sum_{k=1}^{l} \Lambda^k_{\mathrm{SRS}}(\Lambda_k^{\mathrm{DYN}}+2)\langle\alpha_k,\alpha_k\rangle = \tfrac{1}{2}\sum_{k=1}^{l} w^k(a_k+2)\langle\alpha_k,\alpha_k\rangle \ , \tag{5-304a}$$

where $\Lambda_{\mathrm{SRS}} = \{w^1, w^2, \ldots\}$.

Consider, for example the group SU_3. Let the DYN representative of a highest weight be $\Lambda = (a_1, a_2)$. The inverse of the Cartan matrix is $A^{-1} = \frac{1}{3}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$. According to (5-299b), the SRS representative of Λ is

$$\begin{pmatrix} w^1 \\ w^2 \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 2a_1 + a_2 \\ a_1 + 2a_2 \end{pmatrix} \ .$$

Notice that $\langle\alpha_i,\alpha_i\rangle$ is the scalar product of the i-th root with itself, which is scale independent and equal to $\frac{1}{3}$ according to (5-272b). Therefore the eigenvalue of $\mathcal{C}$ in the irrep $\Lambda = (a_1, a_2) \equiv (\lambda,\mu)$ is

$$\mathcal{C}(\lambda,\mu) = \frac{1}{9}\left(\lambda^2+\mu^2+3\lambda+3\mu+\lambda\mu\right) \ , \tag{5-304b}$$

where $(\lambda\mu)$ is the usual label for the SU_3 irreps.

It should be stressed that the Casimir operator in the definition (5-303a) or (5-220a) is in a covariant form, and is thus scale-independent. For example, either for the SU_3 basis $\{H_i, E_\alpha\}$ shown in (5-272a), or for the Cartan–Weyl basis, $H'_i = \sqrt{6}H_i, E'_\alpha = \sqrt{6}E_\alpha$, the Casimir operators are the same and with the same eigenvalue given in (5-304b).

In (5-222) we introduced the Casimir operator C in the coupled form. Using the Cartan–Weyl basis (5-270a), the Casimir operator C can be expressed as

$$C = \sum_i (H_i)^2 + \sum_\alpha E_\alpha E_{-\alpha} \ , \tag{5-305a}$$

which differs from (5-303a) by a multiplicative factor and is scale dependent. For the Cartan–Weyl bases (5-276) of A_l, B_l, C_l and D_l we have the *Casimir operators* in the uncoupled basis

$$C_{U_N} = \sum_\alpha (H_\alpha)^2 + \sum_{\alpha\neq\beta} E_{\alpha\beta}E_{\beta\alpha} \ , \qquad H_\alpha = \hat{n}_\alpha \ , \tag{5-305b}$$

$$\begin{aligned} C_{SU_N} &= \sum_{r=1}^{N-1} (P_0^r)^2 + \sum_{\alpha\neq\beta} E_{\alpha\beta}E_{\beta\alpha} \\ &= \sum_\alpha (H_\alpha)^2 + \sum_{\alpha\neq\beta} E_{\alpha\beta}E_{\beta\alpha} \ , \quad H_\alpha = \hat{n}_\alpha - \frac{\hat{n}}{N} \ , \end{aligned} \tag{5-305c}$$

with P_0^r given in (5-159c).

$$C_{G_N} = \sum_\alpha (H_\alpha)^2 + \sum_{\alpha\beta}{}' X_{\alpha\beta}X_{\beta\alpha} \ , \qquad H_\alpha = \hat{n}_\alpha - \hat{n}_{-\alpha} \ , \tag{5-305d}$$

where the summation range of $\alpha\beta$ is specified by $(\alpha : \beta)$ in (5-170b) and (5-170c).

It can be checked that the Casimir operators (5-305b-d) in uncoupled form are the same as (5-222) in coupled form.

The eigenvalue of the Casimir operator C in (5-305) for the Cartan–Weyl basis is obtained from (5-303b) or (5-304a) by replacing the scalar product $\langle\ \ \rangle$ with $(\ \ )$,

$$C(\Lambda) = (\Lambda, \Lambda + 2R) = \tfrac{1}{2}\sum_{k=1}^{l} w^k(a_k + 2)(\alpha_k, \alpha_k) \ . \tag{5-305e}$$

Noticing that the generators of the Cartan–Weyl basis of SU_3 is $\sqrt{6}$ times those of the standard basis, the eigenvalue for the SU_3 Casimir operator (5-222b) or (5-305c) is six times the value of (5-304b), i. e.

$$C(\lambda, \mu) = \frac{2}{3}\left(\lambda^2 + \mu^2 + 3\lambda + 3\mu + \lambda\mu\right) \ . \tag{5-304c}$$

It should be mentioned that (5-304c) can also be obtained from (5-304a) by replacing $\langle\alpha, \alpha\rangle = \frac{1}{3}$ with $(\alpha, \alpha) = 2$.

5.24.3. The Chevalley basis

In the DYN rep, a weight Λ and a root β are represented by $\Lambda = (a_1, a_2, \ldots, a_l)$ and $\beta = (b_1, b_2, \ldots, b_l)$. The problem we are facing now is to find the l commuting operators $\{H_{\alpha_i}\}$ out of the $\{H_i\}$ so that the a_i and b_i are the quantum numbers of H_{α_i}. Now we show that these operators are

$$H_{\alpha_i} = 2\frac{(\alpha_i, H)}{(\alpha_i, \alpha_i)} = 2\sum_j \frac{(\alpha_i)_j H_j}{(\alpha_i, \alpha_i)} \ . \tag{5-306}$$

Proof: Using (5-306), (5-270a) and (5-283b) we have

$$H_{\alpha_i}|\psi_\Lambda\rangle = a_i|\psi_\Lambda\rangle, \quad a_i = 2\frac{(\alpha_i, \Lambda)}{(\alpha_i, \alpha_i)} \ , \tag{5-307a}$$

$$[H_{\alpha_i}, E_\beta] = b_i E_\beta, \quad b_i = 2\frac{(\alpha_i, \beta)}{(\alpha_i, \alpha_i)} \ . \quad \textbf{QED} \tag{5-307b}$$

From (5-307b) we have

$$[H_{\alpha_i}, E_{\alpha_j}] = A_{ij} E_{\alpha_j} \ , \tag{5-307c}$$

which is consistent with (5-294c). Comparing (5-306) with (5-270a), we see that through proper normalization of the step operators $E_{\pm\alpha_i}$ one has the commutator

$$[E_{\alpha_i}, E_{-\alpha_i}] = H_{\alpha_i} \ . \tag{5-308}$$

The generators satisfying the following commutators are called the *Chevalley basis* of a Lie algebra.

$$[H_{\alpha_i}, H_{\alpha_j}] = 0 \ , \qquad [H_{\alpha_i}, E_{\alpha_j}] = A_{ij} E_{\alpha_j} \ , \tag{5-309a, b}$$

$$[E_{\alpha_i}, E_{-\alpha_i}] = H_{\alpha_i} \ , \quad [E_\beta, E_\gamma] = \pm(p+1)E_{\beta+\gamma} \ , \tag{5-309c, d}$$

where $E_{-\alpha_i} = E_{\alpha_i}^\dagger$, $p = m$ if $(\beta + \gamma)$ is a root, and $p = -1$ if $(\beta + \gamma)$ is not a root, and $m > 0$ is the greatest integer for which $\gamma - m\beta$ is a root (Wybourne 1974).

The step operators associated with the simple roots, $E_{\alpha_1}, \ldots, E_{\alpha_l}$ are called the *generators of the Lie algebra*. Given these generators, the commuting operators H_{α_i} are obtained from (5-308), while the step operators associated with the non–simple roots can be obtained from recursive use of the commutator (5-309d).

There are two methods for finding the Chevalley basis:

1. Use (5-306).

2. (a) Identify the step operators E'_{α_i} associated with the simple roots α_i, which may differ from the E_{α_i} of the Chevalley basis by multiplicative factors. (b) Compute the commutators $[E'_{\alpha_i}, E'_{-\alpha_i}] = H'_{\alpha_i}$, and $[H'_{\alpha_i}, E'_{\alpha_j}] = \mathcal{N}_i A_{ij} E'_{\alpha_j}$. (c) Then the Chevalley basis is: $H_{\alpha_i} = H'_{\alpha_i}/\mathcal{N}_i, E_{\pm\alpha_i} = E'_{\pm\alpha_i}/\sqrt{\mathcal{N}_i}$.

Example: The Chevalley basis of su_3

Method 1. From (5-272), we obtain

$$\begin{aligned} H_\alpha &= \sqrt{3}H_1 + 3H_2 = \hat{n}_1 - \hat{n}_3 \ , \\ H_\beta &= \sqrt{3}H_1 - 3H_2 = \hat{n}_3 - \hat{n}_2 \ , \\ E_\alpha &= C_1^\dagger C_3, \quad E_\beta = C_3^\dagger C_2 \ . \end{aligned} \tag{5-310}$$

Method 2. From (5-272a), we have

$$\begin{aligned} &E'_\alpha = \sqrt{\tfrac{1}{6}}C_1^\dagger C_3, \quad E'_\beta = \sqrt{\tfrac{1}{6}}C_3^\dagger C_2 \ , \\ &H'_\alpha = [E'_\alpha, E'_{-\alpha}] = \tfrac{1}{6}(\hat{n}_1 - \hat{n}_3), \quad H'_\beta = [E'_\beta, E'_{-\beta}] = \tfrac{1}{6}(\hat{n}_3 - \hat{n}_2) \ , \\ &\left[\begin{pmatrix} H'_\alpha \\ H'_\beta \end{pmatrix}, E'_\alpha\right] = \frac{1}{6}\begin{pmatrix} 2 \\ -1 \end{pmatrix} E'_\alpha, \quad \left[\begin{pmatrix} H'_\alpha \\ H'_\beta \end{pmatrix}, E'_\beta\right] = \frac{1}{6}\begin{pmatrix} -1 \\ 2 \end{pmatrix} E'_\beta \ . \end{aligned} \tag{5-311}$$

The Cartan matrix for A_2 is $\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$. Therefore $\mathcal{N}_\alpha = \mathcal{N}_\beta = \frac{1}{6}$, and the Chevalley for su_3 is: $H_\alpha = 6H'_\alpha, H_\beta = 6H'_\beta, E_\alpha = \sqrt{6}E'_\alpha, E_\beta = \sqrt{6}E'_b$ and so on, in agreement with (5-310).

The importance of the Chevalley basis is that the eigenvalues of H_{α_i} in the highest weight state $|\psi^\Lambda\rangle$ give the *Dynkin label* of the irrep.

Ex. 5.9. Construct the Chevalley basis for the Lie algebras B_2 and C_2 using the information given in Exs. 5.4 and 5.6.

5.25. Algorithms for Computing the Roots and Weights

Using the definition of the Dynkin representative of a root or weight vector, Theorems 5.10 and 5.20 can be reformulated as follows:

Theorem 5.25: If there is a root β (or a weight Λ) whose DYN representative is $(m_1, m_2, \ldots, m_l)$, then there exist l strings of roots (weights),

$$\begin{aligned} &\beta, \beta - \theta_i\alpha_i, \ldots, \beta - m_i\alpha_i \ , \quad i = 1, 2, \ldots, l \ , \\ &(\Lambda, \Lambda - \theta_i\alpha_i, \ldots, \Lambda - m_i\alpha_i) \ , \quad \theta_i = \text{sign } (m_i) \ . \end{aligned} \tag{5-312}$$

This theorem provides us with the following two algorithms for roots and weights.

Algorithm 1: The steps for obtaining all positive roots from the Dynkin diagram are:

1. Construct the Cartan matrix A and write down the DYN representatives of the l simple roots,

$$\alpha_j = (A_{1j}, \ldots, A_{lj}) \ , \quad j = 1, 2, \ldots, l \ . \tag{5-313}$$

2. Starting from $\alpha_1 = (A_{11}, A_{21}, \ldots, A_{l1})$, for each *negative coordinate* A_{i1}, we have a string of positive roots,

$$\alpha_1, \alpha_1 + \alpha_i, \alpha_1 + 2\alpha_i, \ldots, \alpha_1 - A_{i1}\alpha_i \ . \tag{5-314}$$

3. Using (5-313), compute the DYN representative of the i–th terminal root,

$$\beta \equiv \alpha_1 - A_{i1}\alpha_i = (b_1, b_2, \ldots, b_l) \ . \tag{5-315}$$

Continue this process until all the coordinates of all the terminal roots are non–negative.

4. Repeat the above steps for the simple roots $\alpha_2, \ldots, \alpha_l$, ignoring in each step the roots which have already appeared in the foregoing steps.

In this way, we can obtain all the positive roots. The result can be checked using Eq. (5-288d).

Example 1: Computing the positive roots of the Lie algebra G_2. From the Cartan matrix (5-281b) we have the simple roots

$$\alpha_1 = (2, -3), \quad \alpha_2 = (-1, 2) \ .$$

From α_1 we find: $\alpha_1, \alpha_1 + \alpha_2, \alpha_1 + 2\alpha_2, \alpha_1 + 3\alpha_2 = (-1, 3)$; $\alpha_1 + 3\alpha_2 + \alpha_1 = 2\alpha_1 + 3\alpha_2 = (1, 0)$. From α_2 we have: $\alpha_2, \alpha_2 + \alpha_1$ (duplicated).

As a check, note that $R = \frac{1}{2}[\alpha_1 + \alpha_2 + (\alpha_1 + \alpha_2) + (\alpha_1 + 2\alpha_2) + (\alpha_1 + 3\alpha_2) + (2\alpha_1 + 3\alpha_2)] = (1, 1)$.

Example 2: Computing the positive roots of the Lie algebra B_3. From the Cartan matrix (5-282b) we have the simple roots

$$\alpha_1 = (2, -1, 0), \quad \alpha_2 = (-1, 2, -2), \quad \alpha_3 = (0, -1, 2) \ .$$

From α_1 we find: $\alpha_1, \alpha_1 + \alpha_2 = (1, 1, -2)$; $\alpha_1 + \alpha_2 + \alpha_3, \alpha_1 + \alpha_2 + 2\alpha_3 = (1, -1, 2)$; $\alpha_1 + 2\alpha_2 + 2\alpha_3 = (0, 1, 0)$.

Similarly from α_2 : $\alpha_2, \alpha_2 + \alpha_3, \alpha_2 + 2\alpha_3 = (-1, 0, 2)$; $\alpha_1 + \alpha_2 + 2\alpha_3$ (duplicated).

From $\alpha_3 : \alpha_3, \alpha_3 + \alpha_2$ (duplicated).
Check: $R = \frac{1}{2}[\alpha_1 + \alpha_2 + \alpha_3 + (\alpha_1 + \alpha_2) + (\alpha_2 + \alpha_3) + (\alpha_1 + \alpha_2 + \alpha_3) + (\alpha_2 + 2\alpha_3) + (\alpha_1 + \alpha_2 + 2\alpha_3) + (\alpha_1 + 2\alpha_2 + 2\alpha_3)] = \frac{1}{2}(5\alpha_1 + 8\alpha_2 + 9\alpha_3) = (1,1,1)$.

Algorithm 2: The steps for computing the complete set of weights are as follows:

1. Same as step 1 for Algorithm 1.

2. Starting from the highest weight $\Lambda = (a_1, a_2, \ldots, a_l)$, for each $a_i > 0$, we have a string of weights

$$\lambda^1(=\Lambda), \lambda^2, \ldots, \lambda^{a_i+1}, \quad \lambda^n = \Lambda - (n-1)\alpha_i . \tag{5-316a}$$

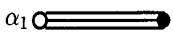
3. Compute the DYN representative of each weight in the string. For each weight $\lambda^m = (m_1, \ldots, m_l)$, if $m_k > 0$, then we have a string of weights

$$\lambda^m, \lambda^m - \alpha_k, \ldots, \lambda^m - m_k\alpha_k . \tag{5-316b}$$

4. Continue the string-searching process for each weight which has not already appeared in the previous steps, until the lowest weight is reached.

5. If the weight system contains the null weight, then by the symmetry between the positive and negative weights, it suffices to compute only the positive weights.

Example 3: Compute the weight system for the irrep $\Lambda = (1,0)$ of G_2.

α_1  α_2 , $A = \begin{pmatrix} 2 & -1 \\ -3 & 2 \end{pmatrix}$, $A^{-1} = \begin{pmatrix} 2 & 1 \\ 3 & 2 \end{pmatrix}$, $\alpha_1 = (2,-3)$, $\alpha_2 = (-1,2)$.

From the first column of A^{-1}, we have $\Lambda = 2\alpha_1 + 3\alpha_2$.

Following the steps of Algorithm 2, we can obtain

$$\begin{array}{llllll}
 & & & & \nearrow & \Lambda - \alpha_1 - 3\alpha_2 \to \Lambda - 2\alpha_1 - 3\alpha_2 \to \\
 & & & & & (2,-3) \qquad (0,0) \\
\Lambda & \to \Lambda - \alpha_1 \to \Lambda - \alpha_1 - \alpha_2 \to \Lambda - \alpha_1 - 2\alpha_2 & & & \searrow & \Lambda - 2\alpha_1 - 2\alpha_2 \to \Lambda - 2\alpha_1 - 3\alpha_2 \to \\
(1,0) & (-1,3) \qquad (0,1) \qquad (1,-1) & & & & (-1,2) \qquad (0,0)
\end{array}$$

$$\begin{array}{llllll}
\to \Lambda - 3\alpha_1 - 3\alpha_2 \searrow & & & & & \\
(-2,3) & & & & & \\
 & \Lambda - 3\alpha_1 - 4\alpha_2 \to \Lambda - 3\alpha_1 - 5\alpha_2 \to \Lambda - 3\alpha_1 - 6\alpha_2 \to \Lambda - 4\alpha_1 - 6\alpha_2 . & & & & \\
\to \Lambda - 2\alpha_1 - 4\alpha_2 \nearrow & (-1,1) \qquad (0,-1) \qquad (1,-3) \qquad (-1,0) & & & & \\
(1,-2) & & & & &
\end{array}$$

(5-317)

The weights $\mathbf{M}$ of a representation Λ can be grouped into *layers* according to their layer index $L(M)$, such as in (5-317), where the weights of the irrep $(1,0)$ of G_2 have 11 layers from the zeroth (the the highest weight) to tenth (the lowest weight) layer. The *level* or *power* of a weight $\mathbf{M}$ is defined as

$$\delta(M) = 2\sum_{i=1}^{l} w^i , \tag{5-318a}$$

where $\{w^1, w^2, \ldots, w^l\}$ is the SRS representative of $\mathbf{M}$. The layer index $L(M)$ can be expressed as

$$L(M) = \frac{1}{2}[\delta(\Lambda) - \delta(M)] . \tag{5-318b}$$

The index $L(M)$ is always an integer and corresponds to the number of simple roots that have to be subtracted from Λ to get M.

The *height* T of an irrep Λ is defined as

$$\text{height of } \Lambda: \qquad T = \delta(\Lambda)\ , \tag{8-318c}$$

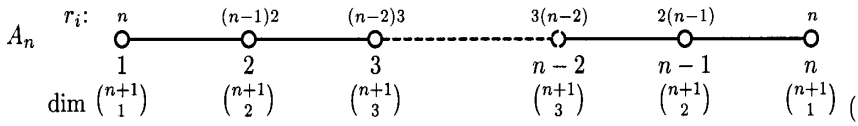
which equals the number of layers minus one. The *height* T can be expressed in terms of the *height* r_i of the i–th basic rep,

$$T = \delta(\Lambda) = \sum_{i=1}^{l} a_i r_i\ , \tag{5-318d}$$

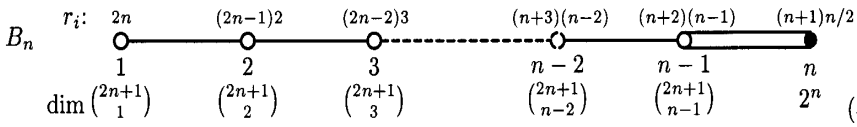
where $(a_1, a_2, \ldots, a_l)$ is the DYN representatives of Λ. According to (5-295c) and (5-318a),

$$r_i = 2\sum_{k=1}^{l} (A^{-1})_{ki}\ . \tag{5-318e}$$

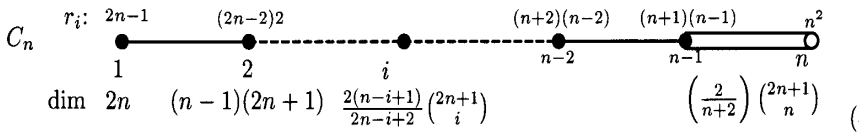
The values of r_i are listed in (5-319).



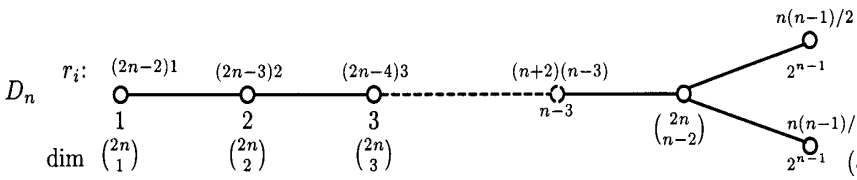
(5-319a)



(5-319b)



(5-319c)



(5-319d)

The height of the irrep (1,0) of G_2 is $T = 2[(A^{-1})_{11} + (A^{-1})_{21}] = 2(2+3) = 10$. The irrep (1,0) is the adjoint rep of G_2 with dimension 14. From (5-317) we can infer that the null weight has the multiplicity two. In general case, Algorithm 2 alone is not enough for determining the multiplicity of weights. For this we need the help of (5-321b).

Similarly, we can find the positive weights for the irrep (0,1) of G_2. Collecting the positive weights for the irreps (1,0) and (0,1), and arranging them as columns of a matrix, we obtain

$$W^{(1)} = \begin{pmatrix} 1 & -1 & 0 & 1 & 2 & -1 \\ 0 & 3 & 1 & -1 & -3 & 2 \end{pmatrix}\ , \quad W^{(2)} = \begin{pmatrix} 0 & 1 & -1 \\ 1 & -1 & 2 \end{pmatrix}\ . \tag{5-319e}$$

$W^{(i)}$ will be referred to as the *weight system* of the basic rep M^i.

Algorithms 1 and 2 are more effective than the methods in Wybourne (1974) and Laskar (1977).

The weights for an irrep (a_1, a_2) of any Lie algebra of rank 2 form "concentric" polygons, which are invariant under the corresponding Weyl group. According to Fig. 5.20 and a Theorem proved in Eq. (8-17), we know that the Weyl groups for $A_2, B_2(C_2)$ and G_2 are the point groups C_{3v}, C_{4v} and C_{6v} respectively. The perimeter of the weights is a polygon consisting of sides with lengths equal to $a_1|\boldsymbol{\alpha}_1|$ and $a_2|\boldsymbol{\alpha}_2|$ alternatively. If both a_1 and a_2 are non-zero, then it is a hexagon, octagon and dodecahedron for A_2, B_2 (or C_2) and G_2, respectively (see Fig. 5.25), and if one of a_1 and a_2 is zero, then it is a triangle, quadrangle and hexagon for A_2, B_2 (or C_2) and G_2, respectively.

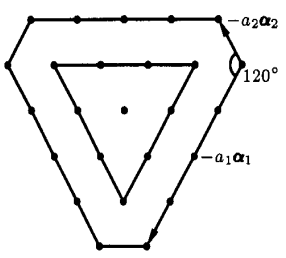


Fig. 5.25-1. Weight diagram for the A_2 irrep (41).

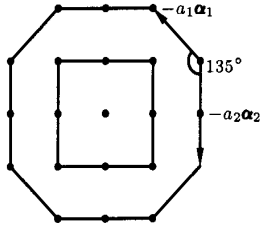


Fig. 5.25-2. Weight diagram for the B_2 irrep (12).

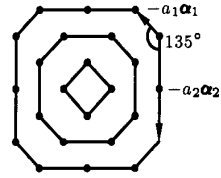


Fig. 5.25-3. Weight diagram for the C_2 irrep (12).

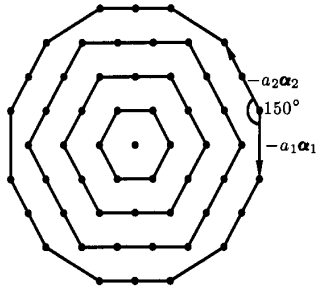


Fig. 5.25-4. Weight diagram for the G_2 irrep (12).

The foregoing procedure exemplified in (5-317) suggests the following diagrammatic method for constructing the weight diagram of the irrep $(a_1 a_2)$ for any Lie algebra of rank 2.

1. In the root diagram draw the simple roots $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$, as well as the basic weights $\mathbf{M}^1$ and $\mathbf{M}^2$.

2. Mark the point $\Lambda = a_1\mathbf{M}^1 + a_2\mathbf{M}^2$. Starting from the two sides $-a_1\boldsymbol{\alpha}_1$ and $-a_2\boldsymbol{\alpha}_2$ originating from the point Λ, we can easily draw the perimeter polygon, as shown in Figs. 5.25.

3. The weight diagram results from a special "chess game." The rules for this "chess" are; (a) the chess piece can only take two kinds of steps, moving ahead through either $-\boldsymbol{\alpha}_1$ or $-\boldsymbol{\alpha}_2$; (b) the chess piece is not allowed to go outside the perimeter. Then starting from the point $\Lambda = a_1\mathbf{M}^1 + a_2\mathbf{M}^2$, all the possible stopover points of the chess piece yield the weight diagram of the irrep $(a_1 a_2)$.

As an example, in Fig. 5.25-5, we show the vectors $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \mathbf{M}^1$ and $\mathbf{M}^2$ of G_2 with solid lines. Figure 5.25-6 is the weight diagram for the irrep (1,0) of G_2 which results from playing the "G_2 chess." As is seen, there is a one-to-one correspondence between Fig. 5.25-6 and Eq. (5-317).

We know that A_2 is a subalgebra of G_2. The simple roots and basic weights of A_2 are also shown in Fig. 5.25-5.

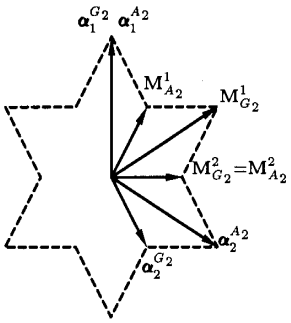


Fig. 5.25-5. The simple roots and basic weights of A_2 and G_2.

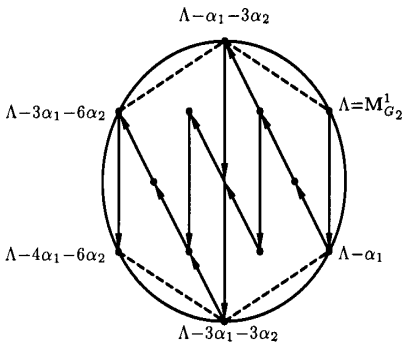


Fig. 5.25-6. The weight diagram of the irrep (1,0) of G_2 resulting from playing "G_2 chess."

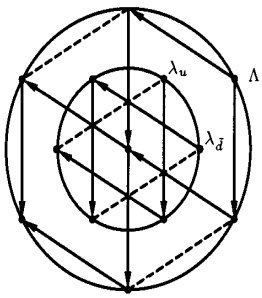


Fig. 5.25-7. The weight diagrams of Fig. 5.25-6 decomposed into three weight diagrams (11), (10) and (01) of A_2 under the "A_2 chess rule."

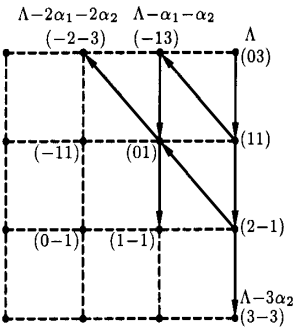


Fig. 5.25-8. The weight diagram of the irrep (03) of B_2.

Now let us look at what happens if, starting from the same point $\Lambda = \mathbf{M}^1_{G_2} = \mathbf{M}^1_{A_2} + \mathbf{M}^2_{A_2}$, we play "$A_2$ chess" instead of "G_2 chess." We immediately see that the chess piece can only reach eight weights (the null weights being counted twice), which constitute the weight diagram of the irrep (11) of A_2, as shown in Fig. 5.25-7. Starting from a weight other than these weights, say λ_u in Fig. 5.25-7, by playing "A_2 chess" again, we obtain a triangle weight diagram, corresponding to the irrep (10) of A_2. Similarly, we obtain another triangle belonging to the irrep (01) of A_2. It is thus seen that the fourteen weights of the irrep (10) of G_2, under the "A_2 chess" rule, group into three disconnected subweight diagrams, corresponding to the subduction

$$\begin{array}{lccl} & G_2 & & A_2 \\ & (10) & \longrightarrow & (11)+(10)+(01) \\ \dim & 14 & = & 8 + 3 + 3 \end{array} . \qquad (5\text{-}320)$$

Freudenthal formula

The multiplicity n_M of a weight M in the irrep Λ can be calculated from the Freudenthal recursive formula (Freudenthal 1969),

$$[(\Lambda+R,\Lambda+R)-(M+R,M+R)]n_M = 2\sum_{\beta>0}\sum_{k=1,2,\ldots}(M+k\beta,\beta)n_{M+k\beta}\ . \tag{5-321a}$$

It can be recast into a more suitable form,

$$(C_\Lambda - C_M)n_M = \sum_{\beta>0}\sum_{k=1,2,\ldots} 2(M+k\beta,\beta)n_{M+k\beta}\ , \tag{5-321b}$$

where the sum over k terminates when $M+k\beta$ exceeds the highest weight, $C_\Lambda(C_M)$ is the eigenvalue of the Casimir operator for the highest weight Λ (the weight M). The eigenvalue C_Λ is given by (5-305e). Suppose $M' = M+k\beta = (m'_1,\ldots,m'_l)$ and $\beta = \{\beta^1,\ldots,\beta^l\}$, then again using (5-301), one has

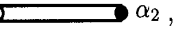
$$(M+k\beta,\beta) = \sum_{i=1}^{l} N_i m'_i \beta^i \equiv (m'_1,\ldots,m'_l)\bullet\{\beta^1,\ldots,\beta^l\}\ . \tag{5-322}$$

According to Theorems 5.21 and 5.17, it suffices to calculate the multiplicities of the weights which are not equivalent to the highest weight, and among the equivalent weights, only the multiplicity of the weight which belongs to the lowest layer. The multiplicities of weights are calculated recursively from low layers to high layers. To calculate the multiplicity of a weight M, we first noted down all the weights M' whose layer indices are lower than that of M. The weights M' are of the form

$$M' = \sum_i b_i\alpha_i + M\ ,$$

with $b_i \geq 0$. Secondly, we check whether $\sum_i b_i\alpha_i = k\beta$, where β is a positive root. If not, then M' is ignored, and if so, its contribution to the sum is calculated by (5-322b).

Example 4: Determine the weights and their multiplicities of the irrep (03) of B_2:

α_1  α_2 , $\quad \alpha_1=(2,-2),\quad \alpha_2=(-1,2),\quad N_1=1,\quad N_2=1/2$.

Using Algorithm 1, it is trivial to get the positive roots:

$$\Sigma^+ : \underset{\{10\},}{\alpha_1}\quad \underset{\{01\},}{\alpha_2}\quad \underset{\{11\},}{\alpha_1+\alpha_2}\quad \underset{\{12\}}{\alpha_1+2\alpha_2}\ . \tag{5-323}$$

Using Algorithm 2, we can find the positive weights listed below, where both the DYN and SRS representatives of each weight are given, which are to be used for computing (5-322).

$$\begin{array}{lllll} & & & & (3,-3)\ \ \alpha_1\ \ (1,-1) \\ & & & \alpha_2 & \{\frac{3}{2}0\}\longrightarrow\{\frac{1}{2}0\} \\ & & (2,-1) & \nearrow & \\ & & \{\frac{3}{2}1\} & \searrow & (01)\ \ \alpha_2\ \ (1,-1) \\ (03) & \alpha_2\ \ (11) & \nearrow & & \alpha_1\ \{\frac{1}{2}1\}\longrightarrow\{\frac{1}{2}0\} \\ \{\frac{3}{2}3\} & \longrightarrow\ \{\frac{3}{2}2\} & \searrow & (-1,3) & \\ & & & \{\frac{1}{2}2\} & \searrow\ (01)\ \ \alpha_1\ \ (-2,3) \\ & & & & \alpha_2\ \{\frac{1}{2}1\}\longrightarrow\{-\frac{1}{2}1\} \end{array}\ . \tag{5-324}$$

The weight diagram is shown in Fig. 5.25-8. From the diagram it is clear that we only need to determine the multiplicity of the weight $M=(01)$, which is in the third layer. Using (5-322),

Eq. (5-321b) reads

$$[C_{(03)} - C_{(01)}]n_{(01)} = 2\Big[(03)\cdot\{12\} + (11)\cdot\{11\} + (-1,3)\cdot\{01\} + (2,-1)\cdot\{10\}\Big],$$
$$8n_{(01)} = 6 + (2+1) + 3 + 4\,,$$

which gives $n_{(01)} = 2$. Hence each of the four inner weights in Fig. 5.25-8 has the multiplicity 2, and the dimension of the irrep (03) of B_2 is equal to $12 + 2 \times 4 = 20$.

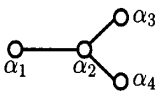
The dominant weight multiplicities for reps of simple Lie algebras have been tabulated by Bremner (1985).

Ex. 5.10. Show that $2\mathbf{R} = \sum_i r_i\boldsymbol{\alpha}_i$ for A_l and D_l; $2\mathbf{R}(B_l) = \sum_i r_i(C_l)\boldsymbol{\alpha}_i$ and $2\mathbf{R}(C_l) = \sum_i r_i(B_l)\boldsymbol{\alpha}_i$.

Ex. 5.11. Find the positive roots and the eigenvalues of the Casimir operators of A_3 and C_3.

Ex. 5.12. Find the weight systems for the irreps (100) and (001) of B_3.

Ex. 5.13. Find the weight systems for the irreps $M^i, i = 1,2,3,4$ of D_4.



Ex. 5.14. Find the multiplicities for the weights of the irrep (11) of A_2 and irrep (200) (the adjoint rep) of C_3.

Ex. 5.15. Draw the weight diagrams for the irreps (10), (01), (11) and (21) of B_2 and C_2.

Ex. 5.16. Draw the weight diagrams for the irreps (30) and (31) of A_2.

Ex. 5.17. Using the diagrammatic method, show that the weight diagram of the irrep (02) of G_2 decomposes in the following way,

$$\begin{array}{ccc} G_2 & & A_2 \\ (02) & \longrightarrow & (20) + (02) + (11) + (10) + (01) + (00)\,. \end{array}$$

Ex. 5.18. Derive the dimension formulas for the irreps of Sp_4, SO_5, SO_6 and SO_8.

Ex. 5.19. Find the DYN representative of the highest weight of the adjoint rep of B_3.

5.26. The Fundamental Weight System

In this section, we deal only with the Lie algebras A_l, B_l, C_l and D_l.

Using Algorithm 2, we can easily obtain the weight systems W, which will be referred to as the *weight matrices* for the fundamental (defining) reps $\mathbf{M}^1$ of A_l, B_l, C_l and D_l.

$$A_l : W = \begin{array}{c} \\ \alpha_1 \\ \alpha_2 \\ \\ \\ \\ \\ \\ \alpha_l \\ \text{[FWS]} \end{array} \begin{array}{c} \begin{array}{ccccc} \lambda^1 & \lambda^2 & & \lambda^l & \lambda^{l+1}\,\text{(DYN)} \end{array} \\ \begin{bmatrix} 1 & -1 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & 0 & 0 \\ \cdot & \cdot & & -1 & 0 \\ 0 & 0 & \cdots & 1 & -1 \end{bmatrix} \end{array}, \qquad B_l : W = \begin{array}{c} \\ \alpha_1 \\ \alpha_2 \\ \\ \\ \\ \\ \\ \alpha_l \\ \text{[FWS]} \end{array} \begin{array}{c} \begin{array}{ccccc} \lambda^1 & \lambda^2 & & \lambda^{l-1} & \lambda^l\,\text{(DYN)} \end{array} \\ \begin{bmatrix} 1 & -1 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & -1 & 0 \\ \cdot & \cdot & & 1 & -1 \\ 0 & 0 & \cdots & 0 & 2 \end{bmatrix} \end{array}, \qquad \text{(5-325a, b)}$$

$$C_l: W = \begin{array}{c} \\ \alpha_1 \\ \alpha_2 \\ \\ \\ \\ \\ \alpha_l \\ \text{[FWS]} \end{array} \begin{array}{c} \begin{array}{ccccc} \lambda^1 & \lambda^2 & & \lambda^{l-1} & \lambda^l \text{ (DYN)} \end{array} \\ \begin{bmatrix} 1 & -1 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & -1 & 0 \\ \cdot & \cdot & & 1 & -1 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix} \end{array} , \qquad D_l: W = \begin{array}{c} l \geq 4 \\ \\ \\ \alpha_1 \\ \alpha_2 \\ \\ \\ \\ \\ \alpha_l \\ \text{[FWS]} \end{array} \begin{array}{c} \begin{array}{ccccc} \lambda^1 & \lambda^2 & & \lambda^{l-2} & \lambda^{l-1} & \lambda^l \text{ (DYN)} \end{array} \\ \begin{bmatrix} 1 & -1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \cdots & \cdot & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & & -1 & 0 & 0 \\ \cdot & \cdot & & 1 & -1 & 0 \\ 0 & 0 & \cdots & 0 & 1 & -1 \\ 0 & 0 & \cdots & 0 & 1 & 1 \end{bmatrix} \end{array} .$$

(5-325c, d)

where the j-th column of W gives the DYN representative of the j-th weight of the irrep $\mathbf{M}^1$,

$$(\lambda^j)^{\text{DYN}} = (W_{1j}, \ldots, W_{\ell j}) , \tag{5-326a}$$

where in the following we use the convention

$$\ell = \begin{cases} l+1, \\ l, \end{cases} \quad \text{for} \begin{cases} A_l \\ B_l, C_l, D_l . \end{cases} \tag{5-326b}$$

That is,

$$\lambda^j = \sum_i W_{ij} \mathbf{M}^i , \tag{5-327a}$$

$$W_{ij} = (\overline{\mathbf{M}}_i, \lambda^j) = 2\frac{(\boldsymbol{\alpha}_i, \lambda^j)}{(\boldsymbol{\alpha}_i, \boldsymbol{\alpha}_i)} . \tag{5-327b}$$

In the process of constructing the weight matrices (5-325), we obtain incidentally,

$$\begin{array}{l} A_l : \\ B_l \quad (C_l) : \boldsymbol{\alpha}_i = \lambda_i - \lambda_{i+1},\ i = \\ D_l : \end{array} \begin{cases} 1, 2, \ldots, l; \\ 1, 2, \ldots, l-1; \quad \boldsymbol{\alpha}_l = \lambda_l \ (\boldsymbol{\alpha}_l = 2\lambda_l) ; \\ 1, 2, \ldots, l-2; \quad \boldsymbol{\alpha}_{l-1} = \lambda_{l-1} - \lambda_l, \\ \qquad\qquad\quad \boldsymbol{\alpha}_l = \lambda_{l-1} + \lambda_l \end{cases} . \tag{5-327c}$$

In other words, the i-th row of the weight matrices W in (7-325) gives the FWS representative of the root $\boldsymbol{\alpha}_i$, $i = 1, \ldots, l$.

5.27. The Fundamental Weight System Rep and the Cartesian Rep

The representation with $(\lambda^1, \ldots, \lambda^\ell)$ as the basis vectors is called the *fundamental weight system* (FWS) representation,

$$\mathbf{v} = \sum_{i=1}^{\ell} v_i^{\text{FWS}} \lambda^i , \tag{5-328a}$$

with the convention that square brackets are used for denoting a FWS representative,

$$[\mathbf{v}]^{\text{FWS}} \equiv [v_1, \ldots, v_\ell]^{\text{FWS}} . \tag{5-328b}$$

From (5-325a) we see that of the $l+1$ weights λ^i for A_l, only l weights are linearly independent,

$$\lambda^1 + \lambda^2 + \ldots + \lambda^{l+1} = 0 . \tag{5-328c}$$

The roots and weights can also be represented in the Cartesian (CAR) representation, the basis vectors of which are just the n mutually orthogonal unit vectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$. We use $|i\rangle$ to denote the i-th single particle state. The basis vectors of the fundamental (or defining) reps and the Cartan subalgebras of A_l, B_l, C_l and D_l are

$$\begin{aligned} A_l: &\quad \{|i\rangle : i = 1, 2, \ldots, l+1\}\,, \qquad H_i = \hat{n}_i - \tfrac{1}{l+1}\sum_{j=1}^{l+1} \hat{n}_j\,, \\ B_l: &\quad \{|i\rangle : i = 0, \pm 1, \pm 2, \ldots, \pm l\}\,, \quad H_i = \hat{n}_i - \hat{n}_{-i}\,, \\ C_l, D_l: &\{|i\rangle : i = \pm 1, \pm 2, \ldots \pm l\}\,, \qquad H_i = \hat{n}_i - \hat{n}_{-i} \end{aligned} \tag{5-329}$$

It is easily seen that

$$\mathbf{H}|i\rangle = \lambda^i |i\rangle\,, \tag{5-330}$$

$$\lambda^i = \begin{cases} \mathbf{e}_i - \frac{1}{l+1}\mathbf{p}, & i = 1, 2, \ldots, l+1 \qquad A_l\,, \\ \mathbf{e}_i, & i = 1, 2, \ldots, l \qquad B_l, C_l, D_l\,, \end{cases} \tag{5-331a, b}$$

where $\mathbf{p}$ is a sum of the $l+1$ unit vectors. The vector $\mathbf{p}$ is perpendicular to the l simple roots $\mathbf{e}_i - \mathbf{e}_{i+1}$, $i = 1, 2, \ldots l$, of A_l, and thus perpendicular to any root or weight vectors $\mathbf{v}$ of A_l,

$$\mathbf{p} = \mathbf{e}_1 + \mathbf{e}_2 + \ldots + \mathbf{e}_{l+1}, \quad (\mathbf{p}, \mathbf{v}) = 0\,. \tag{5-331c}$$

Notice that Eqs. (5-327c), (5-331) and Fig. 5.21-2 are consistent with one another.

The metric tensor for the FWS representation is obtained from (5-331a,b)

$$A_l: \; g^{ij}_{\mathrm{FWS}} = (\lambda^i, \lambda^j) = \begin{cases} l/(l+1)\,, & i = j\,, \\ \text{for} & \\ -1/(l+1)\,, & i \neq j\,, \end{cases} \tag{5-332a}$$

$$B_l, C_l, D_l: \; (\lambda^i, \lambda^j) = \delta_{ij}\,. \tag{5-332b}$$

Hence we see that the CAR representation is identical to the FWS representation for B_l, C_l and D_l. For A_l, the metric tensor of (5-332a) is a singular matrix, therefore we cannot define the dual basis $\{\overline{\lambda}_i\}$ in the usual way. Put differently, for A_l the expansion (5-328a) is not unique. To ensure uniqueness, we impose the condition

$$\sum_{i=1}^{l+1} v_i^{\mathrm{FWS}} = 0\,. \tag{5-333}$$

Substituting (5-331a) into (5-328a), it is seen that under the constraint (5-333), for A_l we also have

$$\mathbf{v} = \sum_{i=1}^{l+1} v_i^{\mathrm{FWS}} \mathbf{e}_i\,, \quad v_i^{\mathrm{FWS}} = (\mathbf{e}_i, \mathbf{v})\,. \tag{5-334a}$$

Due to (5-331a),

$$v_i^{\mathrm{FWS}} = (\mathbf{e}_i, \mathbf{v}) = (\lambda^i, \mathbf{v})\,. \tag{5-334b}$$

Using (5-334a), the scalar product of any root(s) and/or weight(s) of A_l can be easily calculated. So we have reached the important conclusion that for all A_l, B_l, C_l and D_l, the representatives of any root or weight in the FWS and CAR representations are identical,

$$[\mathbf{v}]^{\mathrm{FWS}} = [\mathbf{v}]^{\mathrm{CAR}}\,, \tag{5-335a}$$

and that the scalar product of the root and/or weight vectors can always be calculated from

$$(\mathbf{u},\mathbf{v}) = \sum_{i=1}^{n} u_i^{\mathrm{FWS}} v_i^{\mathrm{FWS}} \ , \tag{5-335b}$$

in spite of the basis (5-331a) for the FWS representation of A_l not being orthonormal.

Using (5-331), (5-327b) can be rewritten as

$$W_{ij} = 2\frac{(\alpha_i,\mathbf{e}_j)}{(\alpha_i,\alpha_i)} = (\overline{\mathbf{M}}_i,\mathbf{e}_j) \ . \tag{5-336}$$

The significance of the FWS representation is that the FWS representative $[l_1,l_2,\ldots,l_\ell]$ of a highest weight Λ is just the *Cartan–Weyl*, or *natural label* for the irreps, namely

$$[\mathbf{v}]^{\mathrm{FWS}} = [\mathbf{v}]^{\text{Cartan-Weyl}} .$$

In the DYN representation, because of (5-326a), Eq. (5-328a) reads

$$v_i^{\mathrm{DYN}} = \sum_{j=1}^{\ell} W_{ij} v_j^{\mathrm{FWS}} \ . \tag{5-337a}$$

Combining (5-299a) and (5-337a), we get

$$(\mathbf{v})^{\mathrm{DYN}} = A\{\mathbf{v}\}_{\mathrm{SRS}} = W[\mathbf{v}]^{\mathrm{FWS}} \ . \tag{5-337b}$$

Equation (5-337b) shows that the weight matrix W is the transformation matrix from the Cartan–Weyl label $[l_1,l_2,\ldots,l_\ell]$ to the Dynkin label $(a_1,a_2,\ldots,a_l)$.

Now we are in a position to examine the meaning of the basic irreps $\mathbf{M}^i$ of A_l, B_l, C_l and D_l. According to (5-284d) and (5-325), we have

$$(\mathbf{M}^1)^{[1^k]}_{\text{h.w.}} = \mathbf{M}^k \ , \quad k = \begin{cases} 1,2,\ldots,l \ , & A_l \ , \\ 1,2,\ldots,l-1 \ , & B_l \ , \\ 1,2,\ldots,l-2 \ , & D_l \ , \end{cases} \tag{5-338a}$$

$$(\mathbf{M}^1)^{[1^k]}_{\text{h.w.}} = \mathbf{M}^k \ , \quad k = 1,2,\ldots,l \qquad C_l \ . \tag{5-338b}$$

According to the dimension formula for the basic reps $\mathbf{M}^i$ shown in (5-319), for the cases of (5-338a), we have

$$\dim\,(\mathbf{M}^1)^{[1^k]} = \dim\,(\mathbf{M}^k) \ . \tag{5-339}$$

Therefore the anti–symmetric reps in (5-338a) are irreducible. Stated differently, the basic rep $\mathbf{M}^k$ for the cases (5-338a) is just the k–th anti–symmetric power of the defining rep $\mathbf{M}^1$,

$$(\mathbf{M}^1)^{[1^k]} = \mathbf{M}^k \ , \quad k = \begin{cases} 1,2,\ldots,l, & A_l \ , \\ 1,2,\ldots,l-1 \ , & B_l \ , \\ 1,2,\ldots,l-2 \ , & D_l \ . \end{cases} \tag{5-340}$$

The reps which can be constructed from the powers of the defining rep $\mathbf{M}^1$ are called the *vector* or *true reps.* The basic rep $\mathbf{M}^l$ of B_l, and the basic reps $\mathbf{M}^{l-1}$ and $\mathbf{M}^l$ of D_l cannot be constructed in this way, and they are referred to as the *spinor reps.*

Remark: For D_4, the basic reps $\mathbf{M}^1, \mathbf{M}^3$ and $\mathbf{M}^4$ are carried into one another by automorphisms of D_4, and we must identify one of them as the defining rep and the other two as spinor reps.

The Kronecker product of two spinor reps gives vector reps, while that of a spinor rep and a vector rep gives spinor reps. For example, we have

$$B_l : (\mathbf{M}^l)^{[2]}_{\text{h.w.}} = (\mathbf{M}^1)^{[1^l]}_{\text{h.w.}} , \quad (\mathbf{M}^l)^{[1^2]}_{\text{h.w.}} = \mathbf{M}^{l-1} , \tag{5-341a}$$

$$D_l : (\mathbf{M}^l)^{[2]}_{\text{h.w.}} = (\mathbf{M}^1)^{[1^l]}_{\text{h.w.}} , \qquad (\mathbf{M}^{l-1} \times \mathbf{M}^l)_{\text{h.w.}} = (\mathbf{M}^1)^{[1^{l-1}]}_{\text{h.w.}} ,$$

$$(\mathbf{M}^{l-1})^{[1^2]}_{\text{h.w.}} = (\mathbf{M}^l)^{[1^2]}_{\text{h.w.}} = \mathbf{M}^{l-2} . \tag{5-341b}$$

In the Dynkin diagrams shown in Fig. 5.21-2, the simple roots are expressed in terms of the Cartesian basis $\{\mathbf{e}_i\}$. Let us define the *root matrix* R whose j–th column gives the CAR representative of α_j which, according to (5-335a), is just the FWS representative of α_j. Therefore,

$$\boldsymbol{\alpha}_j = \sum_{i=1}^{\ell} R_{ij}\mathbf{e}_i = \sum_{i=1}^{\ell} R_{ij}\lambda^i , \tag{5-342a}$$

$$[\boldsymbol{\alpha}_j]^{\text{FWS}} = [R_{1j}, \ldots, R_{\ell j}] , \tag{5-342b}$$

$$R_{ij} = (\mathbf{e}_i, \boldsymbol{\alpha}_j) = (\lambda^i, \boldsymbol{\alpha}_j) . \tag{5-342c}$$

From Eq. (5-327c) we obtain the root matrices.

$$A_l : W = \begin{array}{c} \\ \lambda^1 \\ \lambda^2 \\ \cdot \\ \cdot \\ \cdot \\ \lambda^l \\ \lambda^{l+1} \\ \text{(DYN)} \end{array} \begin{array}{c} \begin{array}{cccccc} \alpha_1 & \alpha_2 & & \alpha_{l-1} & \alpha_l & \text{[FWS]} \end{array} \\ \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ -1 & 1 & \cdots & 0 & 0 \\ 0 & -1 & \cdots & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & 1 & 0 \\ 0 & 0 & \cdots & -1 & 1 \\ 0 & 0 & \cdots & 0 & -1 \end{bmatrix} \end{array} , \quad B_l : R = \begin{array}{c} \\ \lambda^1 \\ \lambda^2 \\ \cdot \\ \cdot \\ \cdot \\ \lambda^{l-1} \\ \lambda^l_{C_l} \\ \text{(DYN)} \end{array} \begin{array}{c} \begin{array}{cccccc} \alpha_1 & \alpha_2 & & \alpha_{l-1} & \alpha_l & \text{[FWS]} \end{array} \\ \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ -1 & 1 & \cdots & 0 & 0 \\ 0 & -1 & \cdots & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & 0 & 0 \\ \cdot & \cdot & \cdots & 1 & 0 \\ 0 & 0 & \cdots & -1 & 1 \end{bmatrix} \end{array} ,$$

(5-343a, b)

$$C_l : R = \begin{array}{c} \\ \lambda^1 \\ \lambda^2 \\ \cdot \\ \cdot \\ \cdot \\ \lambda^{l-1} \\ \lambda^l_{B_l} \\ \text{(DYN)} \end{array} \begin{array}{c} \begin{array}{cccccc} \alpha_1 & \alpha_2 & & \alpha_{l-1} & \alpha_l & \text{[FWS]} \end{array} \\ \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ -1 & 1 & \cdots & 0 & 0 \\ 0 & -1 & \cdots & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & 0 & 0 \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & -1 & 2 \end{bmatrix} \end{array} , \quad \begin{array}{l} D_l : R = \\ l \geq 4 \end{array} \begin{array}{c} \\ \lambda^1 \\ \lambda^2 \\ \cdot \\ \cdot \\ \cdot \\ \lambda^{l-1} \\ \lambda^l \\ \text{(DYN)} \end{array} \begin{array}{c} \begin{array}{cccccc} \alpha_1 & \alpha_2 & & \alpha_{l-1} & \alpha_l & \text{[FWS]} \end{array} \\ \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ -1 & 1 & \cdots & 0 & 0 \\ 0 & -1 & \cdots & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & 0 & 0 \\ \cdot & \cdot & \cdots & 1 & 1 \\ 0 & 0 & \cdots & -1 & 1 \end{bmatrix} \end{array} .$$

(5-343c, d)

Comparing (5-325) with (5-343), one sees that the root matrices are simply related to the weight matrices by

$$R = \tilde{W} , \quad \text{for } A_l \text{ and } D_l , \tag{5-344a}$$

$$R^{B_l} = \tilde{W}^{C_l} , \quad R^{C_l} = \tilde{W}^{B_l} . \tag{5-344b}$$

From (5-326a) and (5-344) one knows that for A_l and D_l, the j–th row of the root matrix R is just the DYN representative of the weight λ^j, while the j–th row of the root matrix of $B_l(C_l)$ is just the DYN representative of the weight λ^j of $C_l(B_l)$. This is explicitly shown in (5-343) by the column headings of the matrices (noting that $\lambda^i_{B_l} = \lambda^i_{C_l}$, for $i = 1, 2, \ldots, l-1$). For example, from (5-343b,c) we have

$$\begin{aligned} B_l: \ & (\lambda^l)^{\mathrm{DYN}} = (0, \ldots, 0, -1, 2) \ , \\ & [\alpha_l]^{\mathrm{FWS}} = [0, 0, \ldots, 0, 1] \qquad (\text{that is, } \alpha_l = \lambda^l) \ ; \end{aligned}$$

$$\begin{aligned} C_l: \ & (\lambda^l)^{\mathrm{DYN}} = (0, \ldots, 0, -1, 1) \ , \\ & [\alpha_l]^{\mathrm{FWS}} = [0, 0, \ldots, 0, 2] \qquad (\text{that is, } \alpha_l = 2\lambda^l) \ . \end{aligned} \tag{5-345}$$

Equation (5-344) can also be proved directly from (5-336) and (5-342c).

From (5-294c) and (5-326), Eq. (5-342a) reads, in the DYN representation,

$$A_{ij} = \sum_{k=1}^{\ell} W_{ik} R_{kj} \ , \quad \text{that is, } A = WR \ . \tag{5-346a}$$

Equation (5-346a) can also be derived from the representation transformation,

$$(\overline{\mathbf{M}}_i, \alpha_j) = \sum_{k=1}^{\ell} (\overline{\mathbf{M}}_i, \mathbf{e}_k)(\mathbf{e}_k, \alpha_j) \ . \tag{5-346b}$$

The inverse of (5-327a) is

$$\mathbf{M}^j = \sum_{i=1}^{\ell} (W^{-1})_{ij} \lambda^i = \sum_{i=1}^{\ell} (W^{-1})_{ij} \mathbf{e}_i \ . \tag{5-347a}$$

Therefore

$$[\mathbf{M}^j]^{\mathrm{FWS}} = [(W^{-1})_{1j}, \ldots, (W^{-1})_{\ell j}] \ , \tag{5-347b}$$

$$(W^{-1})_{ij} = (\mathbf{e}_i, \mathbf{M}^j) = (\lambda^i, \mathbf{M}^j) \ . \tag{5-347c}$$

The inverse of (5-342a) is

$$\lambda^j = \sum_{i=1}^{l} (R^{-1})_{ij} \alpha_i \ , \quad j = 1, 2, \ldots, \ell \ , \tag{5-348a}$$

which implies that

$$\{\lambda^j\}^{\mathrm{SRS}} = \{(R^{-1})_{1j}, \ldots, (R^{-1})_{lj}\} \tag{5-348b}$$

$$(R^{-1})_{ij} = (\overline{\boldsymbol{\alpha}}^i, \lambda^j) = (\overline{\boldsymbol{\alpha}}^i, \mathbf{e}_j) \ . \tag{5-348c}$$

The weight matrix W of A_l in (5-325a) is an $l \times (l+1)$ rectangular matrix. To find its inverse, we employ the following trick. Expressing (5-337a) and (5-333) in one matrix equation, one gets

$$\begin{bmatrix} v_1^{\mathrm{DYN}} \\ \cdot \\ \cdot \\ v_1^{\mathrm{DYN}} \\ 0 \end{bmatrix} = \mathcal{W} \begin{bmatrix} v_1^{\mathrm{FWS}} \\ \cdot \\ \cdot \\ v_l^{\mathrm{FWS}} \\ \\ v_{l+1}^{\mathrm{FWS}} \end{bmatrix} \ , \quad \mathcal{W} = \left[\begin{array}{c} W \\ \hline 1\,1 \ldots 1 \end{array}\right] \ , \tag{5-349}$$

where $\mathcal{W}$ is a $(l+1)\times(l+1)$ matrix. Finding $\mathcal{W}^{-1}$ and deleting its last column, $\left(\frac{1}{l+1},\ldots,\frac{1}{l+1}\right)$, we obtain W^{-1}. The inverse W^{-1} for A_l, B_l, C_l and D_l are given in (5-350), where the relations given by (5-347b), (5-348b) and (5-344) are shown explicitly by the row and column headings of the matrices.

$$A_l : W^{-1} = \begin{array}{c} \\ \lambda^1 \\ \lambda^2 \\ \cdot \\ \cdot \\ \cdot \\ \\ \lambda^l \\ \lambda^{l+1} \\ \{\mathrm{SRS}\} \end{array} \begin{array}{c} \begin{array}{ccccccc} \mathrm{M}^1 & \mathrm{M}^2 & \mathrm{M}^3 & & \mathrm{M}^{l-1} & \mathrm{M}^l & [\mathrm{FWS}] \end{array} \\ \begin{bmatrix} l & l-1 & l-2 & \cdots & 2 & 1 \\ -1 & l-1 & l-2 & \cdots & 2 & 1 \\ -1 & -2 & l-2 & \cdots & \cdot & \cdot \\ \cdot & \cdot & -3 & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & 2 & 1 \\ -1 & -2 & \cdot & & -l+1 & 1 \\ -1 & -2 & -3 & \cdots & -l+1 & -l \end{bmatrix} \end{array} \times \frac{1}{l+1}, \tag{5-350a}$$

$$B_l : W^{-1} = \begin{array}{c} \\ \lambda^1 \\ \lambda^2 \\ \cdot \\ \cdot \\ \cdot \\ \\ \lambda^{l-1} \\ \lambda^l_{C_l} \\ \{\mathrm{SRS}\} \end{array} \begin{array}{c} \begin{array}{ccccccc} \mathrm{M}^1 & \mathrm{M}^2 & & & \mathrm{M}^{l-1} & \mathrm{M}^l & [\mathrm{FWS}] \end{array} \\ \begin{bmatrix} 1 & 1 & \cdots & & 1 & 1/2 \\ 0 & 1 & \cdots & & 1 & 1/2 \\ 0 & 0 & \cdots & & 1 & 1/2 \\ \cdot & \cdot & & & \cdot & \cdot \\ \cdot & \cdot & & & \cdot & \cdot \\ \cdot & \cdot & & & \cdot & \cdot \\ 0 & 0 & \cdots & & 1 & 1/2 \\ 0 & 0 & \cdots & & 0 & 1/2 \end{bmatrix} \end{array}, \tag{5-350b}$$

$$C_l : W^{-1} = \begin{array}{c} \\ \lambda^1 \\ \lambda^2 \\ \cdot \\ \cdot \\ \cdot \\ \\ \lambda^{l-1} \\ \lambda^l_{B_l} \\ \{\mathrm{SRS}\} \end{array} \begin{array}{c} \begin{array}{ccccccc} \mathrm{M}^1 & \mathrm{M}^2 & & & \mathrm{M}^{l-1} & \mathrm{M}^l & [FWS] \end{array} \\ \begin{bmatrix} 1 & 1 & \cdots & & 1 & 1 \\ 0 & 1 & \cdots & & 1 & 1 \\ 0 & 0 & \cdots & & 1 & 1 \\ \cdot & \cdot & & & \cdot & \cdot \\ \cdot & \cdot & & & \cdot & \cdot \\ \cdot & \cdot & & & \cdot & \cdot \\ 0 & 0 & \cdots & & 1 & 1 \\ 0 & 0 & \cdots & & 0 & 1 \end{bmatrix} \end{array}, \tag{5-350c}$$

$$D_l : W^{-1} \quad l \geq 4 = \begin{array}{c} \\ \lambda^1 \\ \lambda^2 \\ \cdot \\ \cdot \\ \cdot \\ \\ \lambda^{l-1} \\ \lambda^l \\ \{\mathrm{SRS}\} \end{array} \begin{array}{c} \begin{array}{cccccccc} \mathrm{M}^1 & \mathrm{M}^2 & & \mathrm{M}^{l-2} & \mathrm{M}^{l-1} & \mathrm{M}^l & [FWS] \end{array} \\ \begin{bmatrix} 1 & 1 & \cdots & 1 & 1/2 & 1/2 \\ 0 & 1 & \cdots & 1 & 1/2 & 1/2 \\ 0 & 0 & \cdots & 1 & 1/2 & 1/2 \\ \cdot & \cdot & & \cdot & \cdot & \\ \cdot & \cdot & & \cdot & \cdot & \\ \cdot & \cdot & & \cdot & \cdot & \\ 0 & 0 & \cdots & 1 & 1/2 & 1/2 \\ 0 & 0 & \cdots & 0 & 1/2 & 1/2 \\ 0 & 0 & \cdots & 0 & -1/2 & 1/2 \end{bmatrix} \end{array}. \tag{5-350d}$$

Notice that the j–th column of W^{-1} gives the Cartan–Weyl label of the j–th basic weight $\mathbf{M}^j$ and that the Cartan–Weyl labels for spinor reps $\mathbf{M}^l$ of B_l and $\mathbf{M}^{l-1}$ and $\mathbf{M}^l$ of D_l involve half–integers.

It is interesting to compare (5-296) [or its explicit forms (5-282) and (5-300)], (5-343) and (5-350), which give the various representatives of the three sets of basic vectors α_j, λ^j and $\mathbf{M}^j$, that is, $(\alpha_j)^{\mathrm{DYN}}$, $\{\mathbf{M}^j\}^{\mathrm{SRS}}$; $[\alpha_j]^{\mathrm{FWS}}$, $(\lambda^j)^{\mathrm{DYN}}$ and $[\mathbf{M}^j]^{\mathrm{FWS}}$, $\{\lambda^j\}^{\mathrm{SRS}}$.

From (5-337b) and (5-346a) we obtain the following transformation relations,

$$\{\mathbf{v}\}_{\mathrm{SRS}} = A^{-1}(\mathbf{v})^{\mathrm{DYN}} = R^{-1}[\mathbf{v}]^{\mathrm{FWS}} , \tag{5-351a}$$

$$[\mathbf{v}]^{\mathrm{FWS}} = W^{-1}(\mathbf{v})^{\mathrm{DYN}} = R\{\mathbf{v}\}_{\mathrm{SRS}} , \tag{5-351b}$$

where

$$R^{-1} = \tilde{W}^{-1}, \quad \text{for } A_l \text{ and } D_l , \tag{5-351c}$$

$$(R^{B_l})^{-1} = (\tilde{W}^{C_l})^{-1} , \quad (R^{C_l})^{-1} = (\tilde{W}^{B_l})^{-1} . \tag{5-351d}$$

In other words, for A_l and D_l, R^{-1} is equal to the transpose of W^{-1}, while R^{-1} of B_l is equal to the transpose of W^{-1} of C_l and vice versa.

Equation (5-351b) shows that W^{-1} is the transformation matrix from the Dynkin label $(a_1, a_2, \ldots a_l)$ to the Cartan–Weyl label $[l_1 l_2 \ldots l_\ell]$.

The dimension formula (5-302) can also be evaluated in the FWS representation. By using (5-276) and (5-335b), and defining

$$p_i = l_i + g_i , \quad [\Lambda]^{\mathrm{FWS}} = [l_1, \ldots, l_\ell] , \quad [\mathbf{R}]^{\mathrm{FWS}} = [g_1, \ldots, g_\ell] , \tag{5-352a}$$

we have the *dimensions* of A_l, B_l, C_l, D_l

$$A_l : \qquad \dim(\Lambda) = \prod_{j>i=1}^{l+1} \left(\frac{p_i - p_j}{g_i - g_j}\right) , \tag{5-352b}$$

$$B_l, C_l : \quad \dim(\Lambda) = \prod_{i=1}^{l} \frac{p_i}{g_i} \prod_{j>i=1}^{l} \left(\frac{p_i - p_j}{g_i - g_j}\right)\left(\frac{p_i + p_j}{g_i + g_j}\right) , \tag{5-352c}$$

$$D_l : \qquad \dim(\Lambda) = \prod_{j>i=1}^{l} \left(\frac{p_i - p_j}{g_i - g_j}\right)\left(\frac{p_i + p_j}{g_i + g_j}\right) . \tag{5-352d}$$

Using (5-351b), (5-350) and (5-288d) we can find

$$\begin{aligned} &A_l : g_i = \frac{l}{2} - i + 1 , \quad B_l : g_i = l - i + \frac{1}{2} , \\ &C_l : g_i = l - i + 1 , \quad D_l : g_i = l - i . \end{aligned} \tag{5-352e}$$

Similarly, from (5-305e) and (5-335b) we can calculate the eigenvalues of the Casimir operators.

$$C = \sum_i \Lambda_i^{\mathrm{FWS}}(\Lambda_i^{\mathrm{FWS}} + 2g_i) = \sum_i l_i(l_i + 2g_i) .$$

The *eigenvalues for the Casimir operators* of SU_N, SO_{2N+1}, Sp_{2N} and SO_{2N} shown in (5-222) or (5-305) are

$$C_{SU_N} = \sum_{i=1}^{N} l_i(l_i + N + 1 - 2i) , \quad C_{SO_{2N+1}} = \sum_{i=1}^{N} l_i(l_i + 2N + 1 - 2i) , \tag{5-352f}$$

$$C_{Sp_{2N}} = \sum_{i=1}^{N} l_i(l_i + 2N + 2 - 2i) , \quad C_{SO_{2N}} = \sum_{i=1}^{N} l_i(l_i + 2N - 2i) . \tag{5-352g}$$

Due to $\sum_{i=1}^{N} l_i = 0$, the eigenvalue C_{SU_N} can be written as

$$C_{SU_N} = \sum_{i=1}^{N} l_i(l_i - 2i) \ . \tag{5-352h}$$

The eigenvalues of the Casimir operators defined in (5-303a) are given in Eqs. (15.4)–(15.12) in Wybourne (1973), and are related to (5-352f,g) as

$$\begin{aligned} C_{SU_N} &= \tfrac{1}{2N} C_{SU_N} \ , & C_{SO_{2N+1}} &= \tfrac{1}{2(2N-1)} C_{SO_{2N+1}} \ , \\ C_{Sp_{2N}} &= \tfrac{1}{4(N+1)} C_{Sp_{2N}} \ , & C_{SO_{2N}} &= \tfrac{1}{4(N-1)} C_{SO_{2N1}} \ . \end{aligned} \tag{5-352i}$$

Putting (5-328) and (5-334) together, we have, for A_l,

$$\mathbf{v} = \sum_{i=1}^{\ell} \mathbf{e}_i(\mathbf{e}_i, \mathbf{v}) = \sum_{i=1}^{\ell} \lambda^i(\lambda^i, \mathbf{v}) = \sum_{i=1}^{\ell} \lambda^i(\mathbf{e}_i, \mathbf{v}) = \sum_{i=1}^{\ell} \mathbf{e}_i(\lambda^i, \mathbf{v}) \ . \tag{5-353a}$$

Consequently, in root or weight space, we have the equalities

$$\begin{aligned} 1 &= \sum_{i=1}^{\ell} |\mathbf{e}_i)(\mathbf{e}_i| = \sum_{i=1}^{\ell} |\lambda^i)(\lambda^i| \\ &= \sum_{i=1}^{\ell} |\lambda^i)(\mathbf{e}_i| = \sum_{i=1}^{\ell} |\mathbf{e}_i)(\lambda^i| \ . \end{aligned} \tag{5-353b}$$

Furthermore we can use (5-331a) in (5-353b) to obtain

$$|\mathbf{p})(\mathbf{p}| = 0 \ , \tag{5-353c}$$

that is, the projection operator $|\mathbf{p})(\mathbf{p}|$ is a null operator in the root or weight space of A_l.

In (5-350a) we see that the matrix W^{-1} for A_l involves fractions, and thus the Cartan–Weyl label $[l_1 l_2 \ldots l_{l+1}]$ for irreps of A_l also involves fractions. To avoid this awkward situation, we introduce a modified FWS representation, denoted FWS′, whose basis vectors are $\lambda^1, \lambda^2, \ldots, \lambda^l$, instead of $\lambda^1, \lambda^2, \ldots, \lambda^{l+1}$. Using (5-328c), we can easily obtain the transformation from the FWS to the FWS′ representation,

$$\mathbf{v} = \sum_{i=1}^{l} v_i^{\mathrm{FWS}'} \lambda^i \ , \tag{5-354a}$$

where

$$v_i^{\mathrm{FWS}'} = v_i^{\mathrm{FWS}} - v_{l+1}^{\mathrm{FWS}} \ , \quad i = 1, 2, \ldots, l \ . \tag{5-354b}$$

Let

$$[\Lambda]^{\mathrm{FWS}'} = [k_1 k_2 \ldots k_l] \ . \tag{5-354c}$$

One has from Eq. (5-354b) that

$$k_i = l_i - l_N, \quad i = 1, 2, \ldots N - 1 \ . \tag{5-354d}$$

In physics we generally use the special unitary group SU_N. However in the presentation of theorems, it is more convenient to use the group U_N. The theory of semi-simple groups applies to the group U_N (Moshinsky 1963), although U_N is not itself a semi-simple group, so long the Cartan subalgebra H_i is defined by

$$U_N : \qquad H_i = \hat{n}_i, \ i = 1, 2, \ldots, N \ . \tag{5-354e}$$

As will be discussed extensively in Sec. 7.2, the irreducible reps of U_N can be labelled by a Young diagram $[\nu] = [\nu_1\nu_2\ldots\nu_N]$ with N rows. Let $|\psi^{[\nu]}_{\text{h.w.}}\rangle$ be the highest weight state of U_N, which has ν_i particles in the ith single–particle state $|i\rangle$, and is characterized by a Young tableau with ν_i $i's$ in the ith row. Applying H_i to the highest weight state we have

$$H_i|\psi^{[\nu]}_{\text{h.w.}}\rangle = \nu_i|\psi^{[\nu]}_{\text{h.w.}}\rangle \ . \tag{5-354f}$$

The eigenvalue of the Casimir operator C_{U_N} for the irrep $[\nu]$ is obtained from (5-352f) with the replacement $l_i \to \nu_i$ (corresponding to the replacement $\hat{n}_i - \frac{\hat{n}}{N} \to \hat{n}_i$, see (5-305b,c)),

$$C_{U_N} = \sum_{i=1}^{N} \nu_i(\nu_i + N + 1 - 2i) \ . \tag{5-355a}$$

Due to (5-222b) the eigenvalue of the Casimir operator of SU_N can be calculated as

$$C_{SU_N} = C_{U_N} - \frac{n^2}{N} \ . \tag{5-355b}$$

It is more convenient to use (5-355a) and (5-355b) instead of (5-352f) to calculate the eigenvalue of C_{SU_N}. For example, from them we can determine the eigenvalue of SU_3, obtaining the same result as in (5-304c).

From (5-305b) and (5-305c) we get the relation between the Cartan–Weyl label $[l_1l_2\ldots l_N]$ of the group SU_N and the partition label $[\nu] = [\nu_1\nu_2\ldots\nu_N]$ of U_N,

$$l_i = \nu_i - \frac{n}{N} \ , \quad n = \sum_{i=1}^{N} \nu_i \ . \tag{5-355c}$$

From (5-354d) and (5-355c) we also have

$$k_i = \nu_i - \nu_N, \quad i = 1, 2, \ldots, N-1 \ . \tag{5-355d}$$

Therefore $[k_1k_2\ldots k_{N-1}]$ represents a Young diagram resulting from deleting the ν_N columns of length N in the Young diagram $[\nu_1\nu_2\ldots\nu_N]$ (compare with (7-71)).

Similar to the case of U_N, we can show that the Cartan–Weyl label $[\Lambda]^{\text{FWS}} = [\sigma] = [\sigma_1\sigma_2\ldots\sigma_l]$ for the vector irreps of B_l and D_l, and any irreps of C_l is the permutational symmetry of a system with the smallest number of particles (denoted by v and called the seniority (Racah 1943,1949, Edmonds 1952) in which the orthogonal (symplectic) symmetry is first encountered.

Let $|\psi^{[\sigma]}_{\text{h.w.}}\rangle$ be the highest weight state of G_N with v particles, which is free of any $\mathcal{S}$ pairs and has σ_i particles in the single–particle state $|i\rangle$, $\sum_{i=1}^{l}\sigma_i = v$. Applying $H_i = \hat{n}_i - \hat{n}_{-i}$ to the highest weight state,

$$H_i|\psi^{[\sigma]}_{\text{h.w.}}\rangle = \sigma_i|\psi^{[\sigma]}_{\text{h.w.}}\rangle \ , \ i = 1, 2, \ldots, l.$$

The eigenvalue of the Casimir operators of G_N for this state is given in (5-352f) and (5-352g) with l_i replaced by σ_i. Let $|\psi^{[\sigma]}_{\mu}\rangle$ be a general state of the irrep $[\sigma]$ free of any $\mathcal{S}$ pairs,

$$\mathcal{S}|\psi^{[\sigma]}_{\mu}\rangle = 0.$$

A state of n particles can be constructed as

$$\mathcal{S}^{\dagger\,(n-v)/2}|\psi^{[\sigma]}_{\mu}\rangle$$

Since $\mathcal{S}^\dagger$ is an invariant of G_N, all the above states belong to the same irrep $[\sigma]$ of G_N.

As with (5-337a), Eq. (5-354a) becomes, in the DYN representation,

$$v_i^{\mathrm{DYN}} = \sum_{j=1}^{l} W_{ij} v_j^{\mathrm{FWS}'} , \tag{5-356a}$$

$$(\mathbf{v})^{\mathrm{DYN}} = W'[\mathbf{v}]^{\mathrm{FWS}'} , \tag{5-356b}$$

where W' is a submatrix of W given in (5-325a), and is precisely the weight matrix of C_l,

$$W' = W^{C_l} . \tag{5-356c}$$

Now Eq. (5-337b) is replaced by

$$(\mathbf{v})^{\mathrm{DYN}} = A\{\mathbf{v}\}_{\mathrm{SRS}} = W'[\mathbf{v}]^{\mathrm{FWS}'} , \tag{5-357a}$$

which in turn implies that (5-351a) becomes

$$\{\mathbf{v}\}_{\mathrm{SRS}} = A^{-1}(\mathbf{v})^{\mathrm{DYN}} = R'^{-1}[\mathbf{v}]^{\mathrm{FWS}'} , \tag{5-357b}$$

where

$$R'^{-1} = A^{-1}W' . \tag{5-358a}$$

Using (5-295b) and (5-336), from (5-358a) we have

$$\begin{aligned}(R'^{-1})_{ik} &= \sum_{j=1}^{l} (\overline{\alpha}^i, \mathbf{M}^j)(\overline{\mathbf{M}}_j, \mathbf{e}_k) = (\overline{\alpha}^i, \mathbf{e}_k) \\ &= (R^{-1})_{ik}, \quad i,k = 1,2,\ldots,l .\end{aligned} \tag{5-358b}$$

Therefore, R'^{-1} results from deleting the last column of R^{-1}.

From (5-357a,b) we obtain

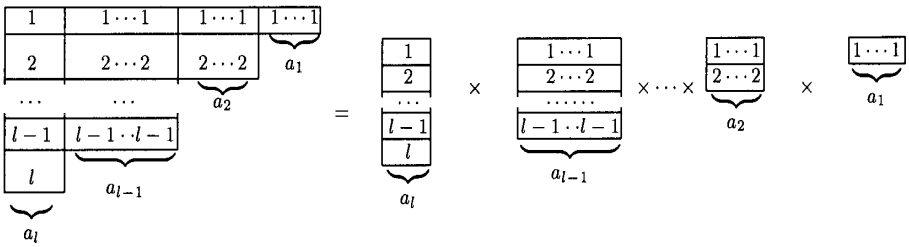
$$[\mathbf{v}]^{\mathrm{FWS}'} = (W^{C_l})^{-1}(\mathbf{v})^{\mathrm{DYN}} = R'\{\mathbf{v}\}_{\mathrm{SRS}} . \tag{5-357c}$$

It should be emphasized that although R'^{-1} is a submatrix of R^{-1}, there is no such simple relation between the matrix R' and R. Indeed, R' has to be found by inverting the matrix R'^{-1}. Equations (5-356) and (5-357) show that the transformation between the FWS′ and DYN representations for A_l is identical with that between the FWS and DYN representations for C_l.

The explicit relation (5-357c) between the FWS′ representative $[k_1, k_2 \ldots k_l]$ and the DYN representative $(a_1 a_2 \ldots a_l)$ of a highest weight Λ is

$$\begin{aligned} k_1 &= a_1 + a_2 + \ldots + a_l , \\ k_2 &= a_2 + \ldots + a_l , \\ &\cdots \\ k_{l-1} &= a_{l-1} + a_l , \\ k_l &= a_l . \end{aligned} \tag{5-357d}$$

The relation (5-357d) between the Young diagram $[k_1 k_2 \ldots k_l]$ and the label $(a_1 a_2 \ldots a_l)$ is illustrated in the following Weyl tableaux of highest weights.



As an example, we list the matrices W, R, W', R' and their inverses for A_2,

$$W = \tilde{R} = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}, \quad W' = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}, \quad \tilde{W}^{-1} = \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 \\ 1 & 1 & -2 \end{pmatrix}, \tag{5-358a}$$

$$W'^{-1} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad R' = \begin{pmatrix} 1 & 1 \\ -1 & 2 \end{pmatrix}, \quad R'^{-1} = \frac{1}{3}\begin{pmatrix} 2 & -1 \\ 1 & 1 \end{pmatrix}, \tag{5-358b}$$

$$WW^{-1} = W'W'^{-1} = W'^{-1}W' = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad W^{-1}W = \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}. \tag{5-358c}$$

Notice that $W^{-1}W$ is not a unit matrix, a peculiarity to be discussed in the next section.

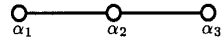
Ex. 5.20. Prove Eqs. (5-338) and (5-341).

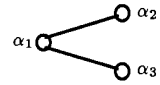
Ex. 5.21. Derive Eq. (5-352).

Ex. 5.22. Show that the Cartan–Weyl irrep labels of SU_4 and SO_6 satisfy the relation shown below.

SU_4 $\qquad$ SO_6 $\qquad$ SU_4 $\qquad$ SO_6

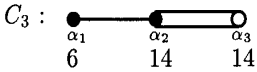
$[l_1 + l_2, l_1 - l_3, l_2 - l_3] \leftrightarrow [l_1 l_2 l_3]$

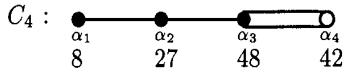




Ex. 5.23. Find the SRS and CAR representatives of the weights for the irrep $\mathbf{M}^1$ of D_4.

Ex. 5.24. The dimensions of the basic reps of C_3 and C_4 are listed below:





Show that

$$C_3 : (\mathbf{M}^1)^{[1^2]} = \mathbf{M}^2 + \mathbf{M}^0, \quad (\mathbf{M}^1)^{[1^3]} = \mathbf{M}^3 + \mathbf{M}^1,$$
$$C_4 : (\mathbf{M}^1)^{[1^2]} = \mathbf{M}^2 + \mathbf{M}^0, \quad (\mathbf{M}^1)^{[1^3]} = \mathbf{M}^3 + \mathbf{M}^1,$$
$$(\mathbf{M}^1)^{[1^4]} = \mathbf{M}^4 + \mathbf{M}^2 + \mathbf{M}^0, \qquad \text{where } \mathbf{M}^0 \text{ is the identity rep.}$$

Ex. 5.25. The irrep of U_N for a system with n electrons and total spin S is labelled by a Young diagram with two columns, $[\nu] = [2^{\frac{n}{2}-S}1^{2S}]$ (see (7-54c)). Show that the eigenvalue of C_{U_N} for the $[\nu]$ is

$$C_{U_N} = \frac{n}{2}(2N + 4 - n) - 2S(S+1). \tag{5-358d}$$

Ex. 5.26. The irrep of SO_N for a system with n electrons is denoted by a Young diagram with two columns, $[l_1 l_2] = [2^{\frac{v}{2}-S}1^{2S}]$ (see (9-59a)). Show that the eigenvalue of C_{SO_N} for the $[l]$ is

$$C_{SO_N} = \frac{v}{2}(2N + 2 - n) - 2S(S+1). \tag{5-358e}$$

Ex. 5.27. The irrep of Sp_N for a system with v nucleons is denoted by a Young diagram with two columns, $[l_1 l_2] = [2^{\frac{v}{2}-\tau}1^{2\tau}]$ (see (9-59c)). Show that the eigenvalue of C_{Sp_N} for the $[l]$ is

$$C_{Sp_N} = \frac{v}{2}(2N + 6 - n) - 2\tau(\tau+1). \tag{5-358f}$$

5.28. Comparing the Different Representations

We have introduced various representations for the classical groups. They are the SRS and DYN representations for all classical Lie groups, and the extra two representations, the FWS and CAR representations for A_l, B_l, C_l and D_l. The SRS representation has the advantage of being intuitive and the SRS representative of a weight M is closely related to the power $\delta(M)$ of the weight, $\delta(M) = 2\sum_{i=1}^{l} w^i$. The DYN representation is especially important since the two basic theorems on roots and weights take very simple forms in the DYN representation and thus it is most suitable for computing the root and weight systems. The SRS and DYN representations are complementary or dual to each other, since their bases are dual bases up to a normalization factor. For B_l, C_l and D_l, the FWS representation coincides with the CAR representation, with the obvious merit that its basis vectors are orthonormal. For A_l, the FWS representation is similar but not identical with the CAR representation, as shown in (5-332a), (5-353a) and (5-335). The FWS representation has the virtue that its "effective metric tensor" is a unit matrix, as seen from (5-335b), but has the drawback that the representative of a weight is not a set of integers or half–integers. Finally there is a fifth representation only for A_l, the modified FWS, or FWS′ representation. The FWS′ representation has the virtue that a weight is represented by a set of integers, which is just the partition if the weight is a highest weight. However the "effective metric tensor" is no longer a unit matrix, that is,

$$(\mathbf{u}, \mathbf{v}) \neq \sum_{i=1}^{l} u_i^{\mathrm{FWS}'} v_i^{\mathrm{FWS}'} \ . \tag{5-359}$$

Despite the striking similarities between the FWS and CAR representations, there are subtle and profound differences between the bases of the two representations, which can be misleading. For example, from (5-336), it seems that we might have

$$\mathbf{e}_j = \sum_{i=1}^{l} W_{ij} \mathbf{M}^i = \sum_{i=1}^{l} (\overline{\mathbf{M}}_i, \mathbf{e}_j) \mathbf{M}^i \ . \tag{5-360}$$

Comparing this with (5-327a), it appears that for A_l we also have $\lambda^i = \mathbf{e}_i$ which contradicts (5-331a). In fact, Eq. (5-360) is false, since if it were true, then in the $(l+1)$-dimensional space $(\mathbf{e}_1, \ldots, \mathbf{e}_{l+1})$ we would have

$$\sum_{i=1}^{l} |\mathbf{M}^i)(\overline{\mathbf{M}}_i| = 1 \ , \tag{5-361}$$

which means that the l basic vectors $\mathbf{M}^1, \ldots, \mathbf{M}^l$ form a complete set of vectors in the $(l+1)$-dimensional space. But this is impossible. In fact, (5-361) holds only in the l-dimensional root or weight space spanned by $(\lambda^1, \ldots, \lambda^{l+1})$, or $(\alpha_1, \ldots \alpha_l)$, or $(\mathbf{M}^1 \ldots, \mathbf{M}^l)$.

Using (5-336) and (5-347c), we have

$$(WW^{-1})_{ik} = \sum_{j=1}^{l+1} (\overline{\mathbf{M}}_i, \mathbf{e}_j)(\mathbf{e}_j, \mathbf{M}^k) = (\overline{\mathbf{M}}_i, \mathbf{M}^k) = \delta_{ik}, \quad i, k = 1, 2, \ldots, l \ . \tag{5-362a}$$

On the other hand,

$$(W^{-1}W)_{ik} = \sum_{j=1}^{l} (\mathbf{e}_i, \mathbf{M}^j)(\overline{\mathbf{M}}_j, \mathbf{e}_k) \neq (\mathbf{e}_i, \mathbf{e}_k) = \delta_{ik}, \quad i, k = 1, 2, \ldots, l+1 \ , \tag{5-362b}$$

since

$$|\mathbf{M}^j)(\overline{\mathbf{M}}_j| \begin{cases} \neq 1, & \text{in the space}(\mathbf{e}_1, \ldots, \mathbf{e}_{l+1}) \ , \\ = 1, & \text{in the space}(\lambda^1, \ldots, \lambda^{l+1}) \ . \end{cases}$$

However, by (5-347c) and (5-327b), we have

$$(W^{-1}W)_{ik} = \sum_{j=1}^{l} (\lambda^i, \mathrm{M}^j)(\overline{\mathrm{M}}_j, \lambda^k) = (\lambda^i, \lambda^k) = g^{ik}_{\mathrm{FWS}} \,. \tag{5-363}$$

An example of (5-363) is given in (5-358c). Therefore, although WW^{-1} is an $l \times l$ unit matrix, $W^{-1}W$ is not a unit matrix. Equation (5-363) can also be written as

$$W^{-1}W = I - \frac{1}{n}N, \quad N = \begin{bmatrix} 1\,1 \cdots 1 \\ 1\,1 \cdots 1 \\ \vdots\ \vdots\ \ \vdots \\ 1\,1 \cdots 1 \end{bmatrix}, \quad n = l + 1 \,, \tag{5-364}$$

where I is an $n \times n$ unit matrix. According to (5-328c), $[\mathbf{v}]^{\mathrm{FWS}} = [11, \ldots 1]$ is a null vector, so that N is equivalent to a null matrix. Hence we see that although $W^{-1}W$ is not a unit matrix in appearance, it is equivalent to an $n \times n$ unit matrix.

A more rigorous way to treat the representation transformation for A_l is to artificially expand the l-dimensional root space into a "pseudo" n-dimensional space, with the convention that $\mathrm{M}^n = \boldsymbol{\alpha}_n = 0, v^n_{\mathrm{SRS}} = v^{\mathrm{DYN}}_n = 0$. Define the $n \times n$ matrices,

$$\mathcal{W} = \tilde{\mathcal{R}} = \left[\begin{array}{c} W \\ \hline 1\,1 \ldots 1 \end{array}\right], \quad \mathcal{R}^{-1} = \tilde{\mathcal{W}}^{-1} = \left[\begin{array}{c} R^{-1} \\ \hline \frac{1}{n}\,\frac{1}{n} \ldots \frac{1}{n} \end{array}\right],$$

$$\mathcal{A} = \left[\begin{array}{c|c} A & \\ \hline & n \end{array}\right]\,., \quad \mathcal{A}^{-1} = \left[\begin{array}{c|c} A^{-1} & \\ \hline & n^{-1} \end{array}\right]\,. \tag{5-365}$$

We have

$$A = \mathcal{W}\mathcal{R} \,, \quad \mathcal{W}\mathcal{W}^{-1} = \mathcal{W}^{-1}\mathcal{W} = \mathfrak{S} \,, \tag{5-366}$$

where $\mathfrak{S}$ is an $n \times n$ unit matrix. Then in place of (5-337b), in the "pseudo" n-dimensional space we have

$$(\mathbf{v})^{\mathrm{DYN}} = \mathcal{A}\{\mathbf{v}\}_{\mathrm{SRS}} = \mathcal{W}[\mathbf{v}]^{\mathrm{FWS}} \,. \tag{5-367}$$

From (5-366) and (5-367), we can easily obtain the other two relations corresponding to (5-351a,b). By (5-333) and the special structure of the matrices in (5-365), as well as the convention that $v^n_{\mathrm{SRS}} = v^{\mathrm{DYN}}_n = 0$, we see that the following equivalences hold,

$$\mathcal{R} \doteq R, \quad \mathcal{R}^{-1} \doteq R^{-1}, \quad \mathcal{W} \doteq W, \quad \mathcal{W}^{-1} \doteq W^{-1}, \quad \mathcal{A} \doteq A, \quad \mathcal{A}^{-1} \doteq A^{-1} \,, \tag{5-368}$$

where "$\doteq$" means equivalence, that is for example $\mathcal{R}$ and R have the same effect. Thus we are led back to Eqs. (5-337b) and (5-351a,b). Introducing the column vectors

$$\mathbf{M} = \begin{bmatrix} \mathrm{M}^1 \\ \vdots \\ \mathrm{M}^l \end{bmatrix}, \quad \boldsymbol{\alpha} = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_l \end{bmatrix}, \quad \boldsymbol{\lambda} = \begin{bmatrix} \lambda^1 \\ \vdots \\ \lambda^\ell \end{bmatrix}, \tag{5-369}$$

the transformations between the coordinate vectors and that between the basis vectors for the

three representations are summarized in the following:

$$\begin{aligned} 1.\ (\mathbf{v})^{\mathrm{DYN}} = A\{\mathbf{v}\}_{\mathrm{SRS}} &= W[\mathbf{v}]^{\mathrm{FWS}}\ , \\ \mathbf{M} = \tilde{A}^{-1}\boldsymbol{\alpha} &= \tilde{W}^{-1}\boldsymbol{\lambda}\ , \end{aligned} \tag{5-370}$$

$$\begin{aligned} 2.\ \{\mathbf{v}\}_{\mathrm{SRS}} = A^{-1}(\mathbf{v})^{\mathrm{DYN}} &= R^{-1}[\mathbf{v}]^{\mathrm{FWS}}\ , \\ \boldsymbol{\alpha} = \tilde{A}\mathbf{M} &= \tilde{R}\,\boldsymbol{\lambda}\ , \end{aligned} \tag{5-371}$$

$$\begin{aligned} 3.\ [\mathbf{v}]^{\mathrm{FWS}} = W^{-1}(\mathbf{v})^{\mathrm{DYN}} &= R\{\mathbf{v}\}_{\mathrm{SRS}}\ , \\ \boldsymbol{\lambda} = \tilde{W}\mathbf{M} &= \tilde{R}^{-1}\boldsymbol{\alpha}\ . \end{aligned} \tag{5-372}$$

The *Cartan-Weyl label* $[\mathbf{v}]^{\mathrm{FWS}}$ and *Dynkin label* $(\mathbf{v})^{\mathrm{DYN}}$ are the two most commonly used labelling schemes for irreps of Lie groups.

For A_l and D_l, the transformations take the more symmetric form,

$$(\mathbf{v})^{\mathrm{DYN}} = W[\mathbf{v}]^{\mathrm{FWS}}\ ,\quad [\mathbf{v}]^{\mathrm{FWS}} = \tilde{W}\{\mathbf{v}\}_{\mathrm{SRS}}\ , \tag{5-373a}$$

$$\boldsymbol{\alpha} = W\boldsymbol{\lambda}\ ,\qquad \boldsymbol{\lambda} = \tilde{W}\mathbf{M}\ . \tag{5-373b}$$

The three representatives for $\alpha_j, \mathbf{M}^j$ and λ^j are listed below.

	SRS	DYN	FWS
α_j :	$\{0\ldots010\ldots0\}$,	$(A_{1j}\ldots A_{lj})$,	$[R_{1j}\ldots R_{lj}]$.
$\mathbf{M}^j$:	$\{(A^{-1})_{1j}\ldots(A^{-1})_{lj}\}$,	$(0\ldots010\ldots0)$,	$[(W^{-1})_{1j}\ldots(W^{-1})_{lj}]$.
λ^j :	$\{(R^{-1})_{1j}\ldots(R^{-1})_{lj}\}$,	$(W_{1j}\ldots W_{lj})$,	$[0\ldots010\ldots0]$.

The labelling schemes for simple roots and irreps of the classical Lie algebras have been studied by Wybourne (1974), Laskar (1977) and King (1981). Equations (5-371)-(5-373) and (5-357) here cover Eqs. (12.22)–(12.24), and (12.28) of Wybourne (1974), and Table 9 of King (1981). Extending the CAR representation to the case of the exceptional Lie algebras is possible. However, the choice of a particular Cartesian representation for exceptional Lie algebra is not unique (King 1981).

All results in the previous sections about roots and weights are implemented in the algebraic software "Killing" (Bernardes 2000), which was designed to manipulate elements of representation theory for classical, exceptional and deformed Lie algebra.

5.29. The Characters and CG Series of Lie Algebras

5.29.1. The characters of Lie groups

The character $\chi(\Lambda,\phi)$ for the irrep Λ of a semi-simple Lie group is a function of the l class parameters $\phi^1,\phi^2,\ldots\phi^l$ (Weyl, 1946),

$$\chi(\Lambda,\phi) = \sum_{\mathbf{m}} \gamma^{\Lambda}(\mathbf{m}) \exp\left(i\sum_j m_j\phi^j\right)\ , \tag{5-374}$$

where the sum extends over all distinct weights $[\mathbf{m}] = [m_1 m_2\ldots]$ (in the FWS representation) of the rep Λ and where $\gamma^{\Lambda}(\mathbf{m})$ is the multiplicity of each weight. Weyl has shown that the character (5-374) can be calculated by

$$\chi(\Lambda,\phi) = \frac{\xi(K,\phi)}{\xi(R,\phi)}\ ,\quad K = \Lambda + R\ , \tag{5-375a}$$

$$\xi(K,\phi) = \sum_S \delta_S \exp\left[i \sum_j (SK)_j \phi^j\right] , \tag{5-375b}$$

where R is defined in (5-288c), the sum runs over all the elements S of the Weyl reflection group, and δ_S is $+1$ (-1) if the number of reflections is even (odd).

For the Lie algebras A_l, B_l, C_l and D_l, the characters have simple explicit expressions (Weyl, 1946),

$$\chi(\Lambda,\phi) = \frac{\det|f(p_i\phi^k)|}{\det|f(g_j\phi^k)|} \tag{5-376a}$$

where both the numerator and denominator are determinants of $n \times n$ matrices ($n = l+1$ for A_l, and $n = l$ for B_l, C_l and D_l) with matrix elements $f(p_j\phi^k)$ and $f(g_j\phi^k)$ in the j–th row and k–th column. We gave p_j and g_j in (5-352), and the function $f(p_j\phi^k)$ has the following form.

	A_l	B_l and C_l	D_l (for $l_n = 0$)
$f(p_j\phi^k)$	$\exp(ip_j\phi^k)$	$\sin(p_j\phi^k)$	$\cos(p_j\phi^k)$

The character for the spinor representation $l_n \neq 0$) of D_l is (Boerner, p. 248)

$$\chi(\Lambda,\phi) = \frac{\det|\cos(p_j\phi^k)| + \det|i\sin(p_j\phi^k)|}{\det|\cos(g_j\phi^k)|} . \tag{5-376b}$$

Using $p_i = l_i + g_i$ and (5-355c), the character for the SU_n group can be written in terms of the partition $[\nu]$,

$$\chi([\nu],\phi) = \exp\left[-i\sum_{j=1}^n \nu_j\right] \frac{\det\left|\exp\left[i(\nu_j+g_j)\phi^k\right]\right|}{\det|\exp(ig_j\phi^k)|} . \tag{5-376c}$$

5.29.2. The CG series of Lie groups

The CG series of a Lie algebra can be determined from the weight theorems. The CG series is denoted by

$$\Lambda \times \Lambda' = \sum_{\Lambda''} (\Lambda\Lambda'\Lambda'')(\Lambda'') . \tag{5-377}$$

The coefficients $(\Lambda\Lambda'\Lambda'')$ can be calculated in the following way:

From (5-284a) and (5-377) we know that the CSW of the Kronecker product $(\Lambda \times \Lambda')$, $\Delta(\Lambda \times \Lambda')$, is decomposed as follows:

$$\Delta(\Lambda \times \Lambda') = \sum_{\Lambda''} \oplus (\Lambda\Lambda'\Lambda'')\Delta(\Lambda'') . \tag{5-378}$$

The highest weight of $\Delta(\Lambda \times \Lambda')$ is

$$\Lambda_1'' = \Lambda + \Lambda' , \tag{5-379}$$

and is necessarily simple. This implies that $(\Lambda\Lambda'\Lambda_1'') = 1$. Using Algorithm 2, we can find the CSW $\Delta(\Lambda_1'')$ for the irrep Λ_1''. Subtracting $\Delta(\Lambda_1'')$ from $\Delta(\Lambda \times \Lambda')$, we get the set of weights $\Delta_1 = \Delta(\Lambda \times \Lambda') - \Delta(\Lambda_1'')$. Using Theorem 5.22 we can find the highest weight Λ_2'' in the set Δ_1. Suppose that the number of the weight Λ_2'' in Δ_1 is m_2, then $(\Lambda\Lambda'\Lambda_2'') = m_2$. Find the CSW $\Delta(\Lambda_2'')$ and subtract $m_2\Delta(\Lambda_2'')$ from Δ_1 to get Δ_2. If the highest weight Λ_3'' occurs m_3 times in Δ_2, then $(\Lambda\Lambda'\Lambda_3'') = m_3$. Continue this process, until all the weights in $\Delta(\Lambda \times \Lambda')$ are exhausted.

Example: Find the CG series for $(10)\times$ (01) of A_2. It is convenient to work in the DYN representation. The CSW for the irreps (10) and (01) are

$$\Delta(10) = \{(10),(-1,1),(0,-1)\}, \quad \Delta(01) = \{(01),(1,-1),(-1,0)\} .$$

Thus we have

$$((10) \times (01)) = \{(11), (2,-1), (00)^3, (-1,2), (-2,1), (1,-2), (-1,-1)\} .$$

The highest weight here is (11), with the CSW

$$(11) = \{(11), (2,-1), (00)^2, (-1,2), (-2,1), (1,-2), (-1,-1)\} ,$$

while

$$\Delta((10) \times (01)) - \Delta(11) = (00) .$$

Therefore the CG series is

$$(10) \times (01) = (11) + (00) .$$

The foregoing method is straightforward but tedious and becomes intractable for irreps of high dimensions. A simpler method is provided by Weyl (1946) which is based on the decomposition, (3-273b), of the character $\chi(\Lambda, \phi)\chi(\Lambda', \phi)$ of the Kronecker product rep. Using the expression (5-375a) for $\chi(\Lambda, \phi)$ and (5-374) for $\chi(\Lambda'; \phi)$, it can be shown (Weyl 1946, Judd 1963 and Racah 1964) that

$$\chi(\Lambda, \phi)\chi(\Lambda', \phi) = \sum_{\mathbf{m}'} \gamma^{\Lambda'}(\mathbf{m}')\chi(\Lambda + \mathbf{m}', \phi) , \tag{5-380a}$$

$$\chi(\Lambda + \mathbf{m}', \phi) = \chi(l_1 + m_1', l_2 + m_2', \ldots, \phi) , \tag{5-380b}$$

where the sum is extended over all distinct weights $[\mathbf{m}'] = [m_1' m_2' \ldots]$ of the irrep Λ'. Notice that the symbol $[l_1 + m_1', l_2 + m_2', \ldots]$ may not be a permissible irrep label. In such cases, we need to use Eq. (5-376) to express $\chi(\Lambda + \mathbf{m}', \phi)$ in an acceptable form. For example, for the group SO_5 from (5-352e) we have $g_1 = \frac{3}{2}, g_2 = \frac{1}{2}$, and from (5-376b) we have

$$\chi(l_1, l_2, \phi) = \begin{vmatrix} \sin\left(l_1 + \frac{3}{2}\right)\phi^1 & \sin\left(l_1 + \frac{3}{2}\right)\phi^2 \\ \sin\left(l_2 + \frac{1}{2}\right)\phi^1 & \sin\left(l_2 + \frac{1}{2}\right)\phi^2 \end{vmatrix} \Bigg/ \begin{vmatrix} \sin\left(\frac{3}{2}\right)\phi^1 & \sin\left(\frac{3}{2}\right)\phi^2 \\ \sin\left(\frac{1}{2}\right)\phi^1 & \sin\left(\frac{1}{2}\right)\phi^2 \end{vmatrix} \tag{5-381}$$

From (5-381) we immediately know that

$$\chi(l_1, l_2) = -\chi(l_2 - 1, l_1 + 1) = -\chi(l_1, -l_2 - 1) = -\chi(-l_1 - 3, l_2) , \tag{5-382a}$$

$$\chi(l_1, l_1 + 1) = \chi\left(l_1, -\tfrac{1}{2}\right) = 0 . \tag{5-382b}$$

Example: Find the CG series for $\left[l_1 \tfrac{1}{2}\right] \times [11]$ of the group SO_5.

The irrep [11] of SO_5 has 10 weights, $\mathbf{m}' = \pm[11], \pm[10], \pm[01], \pm[1,-1], [00]^2$. Using (5-380) and (5-382) we get

$$\left[l_1 \tfrac{1}{2}\right] \times [11] = \left[l_1 + 1, \tfrac{3}{2}\right] + \left[l_1 \tfrac{3}{2}\right] + \left[l_1 - 1, \tfrac{3}{2}\right] + \left[l_1 + 1, \tfrac{1}{2}\right] + 2\left[l_1 \tfrac{1}{2}\right] + \left[l_1 - 1, \tfrac{1}{2}\right] . \tag{5-382c}$$

Ex. 5.28. Find the CG series (10) × (10) of B_2.
Ex. 5.29. Find the CG series (01) × (01) and (10) × (01) of G_2.
Ex. 5.30. Compute the CG series [21] × [21] of SU_3
Ex. 5.31. Compute the CG series for [210]×[100] of Sp_6 and SO_7.
Ex. 5.32. Compute the CG series for [1000] × $\left[\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\right]$ of SO_8.

Chapter 6
The Rotation Group

The rotation group SO_3 in three–dimensional space is the simplest non–Abelian Lie group and the one most familiar to us. The rep theory of SO_3 can be easily understood from the CSCO approach. Indeed the new approach to the rep theory of finite groups has its origins in the analysis of the group SO_3. The purpose of this chapter is to use the group SO_3 as an example to illustrate how the rep theory for finite groups and Lie groups can be unified by the CSCO approach. We shall avoid most subjects specifically relating to SO_3, since they are treated in many good texts. Readers are referred to texts such as Rose (1957), Edmonds (1957), Fano (1959), and Biedenharn (1984), regarding other topics in the rep theory of the rotation group, such as angular momentum theory, D functions, CG coefficients and irreducible tensors.

In Sec. 5.10 we introduced the *double rotation groups* $SO_2^\dagger$ or $SO_3^\dagger$. Written out explicitly, we have

$$SO_2 = \{e^{-i\varphi J_z} : 0 \le \varphi \le 2\pi\} , \tag{6-1a}$$

$$SO_2^\dagger = \{e^{-i\varphi J_z} : 0 \le \varphi \le 4\pi\} , \tag{6-1b}$$

$$\begin{aligned} SO_3 &= \{R_{\mathbf{n}(\theta'\varphi')}(\varphi) : 0 \le \theta' \le \pi, \quad 0 \le \varphi' \le 2\pi, \quad 0 \le \varphi \le \pi\} \\ &= \{R(\alpha\beta\gamma) : 0 \le \alpha, \gamma \le 2\pi, \quad 0 \le \beta \le \pi\} , \end{aligned} \tag{6-1c}$$

$$\begin{aligned} SO_3^\dagger &= \{R_{\mathbf{n}(\theta'\varphi')}(\varphi) : 0 \le \theta' \le \pi, \quad 0 \le \varphi' \le 2\pi, \quad 0 \le \varphi \le 2\pi\} \\ &= \{R(\alpha\beta\gamma) : 0 \le \alpha \le 2\pi, \ 0 \le \beta \le \pi, \ 0 \le \gamma \le 4\pi\} . \end{aligned} \tag{6-1d}$$

In the following we shall discuss the reps for both the rotation group and the double rotation group.

6.1. The Differential Operators $J_{x,y,z}$ and $\overline{J}_{x,y,z}$ in Group Parameter Space

Using (5-177b) and the combination law of group parameters (5-23), we can find the differential form for the infinitesimal operators J_x, J_y and J_z in group parameter space. We choose the Euler angle α, β and γ as parameters, and consider the product of two successive rotations

$$R(\alpha_3\beta_3\gamma_3) = R(\alpha_2\beta_2\gamma_2)R(\alpha_1\beta_1\gamma_1) .$$

However the combination law for the Euler angles α, β and γ,

$$(\alpha_3\beta_3\gamma_3) = \varphi(\alpha_1\beta_1\gamma_1, \alpha_2\beta_2\gamma_2) ,$$

is not easy to work out explicitly. Using the homomorphism of SU_2 to SO_3, one can obtain the combination law for the SO_3 group parameters in terms of those for the SU_2 group parameters. Let us therefore consider the product of two SU_2 transformations

$$\begin{pmatrix} c_0 - ic_3, & -c_1 - ic_2 \\ c_1 - ic_2, & c_0 + ic_3 \end{pmatrix} = \begin{pmatrix} b_0 - ib_3, & -b_1 - ib_2 \\ b_1 - ib_2, & b_0 + ib_3 \end{pmatrix} \begin{pmatrix} a_0 - ia_3, & -a_1 - ia_2 \\ a_1 - ia_2, & a_0 + ia_3 \end{pmatrix} . \tag{6-2a}$$

From (5-188) one gets the relations between the group parameters of SO_3 and SU_2:

$$\begin{aligned} a_0 &= \cos\frac{\beta_1}{2}\cos\frac{\alpha_1+\gamma_1}{2}\,, & a_1 &= \sin\frac{\beta_1}{2}\cos\frac{\gamma_1-\alpha_1}{2}\,, \\ a_2 &= \sin\frac{\beta_1}{2}\sin\frac{\gamma_1-\alpha_1}{2}\,, & a_3 &= \cos\frac{\beta_1}{2}\sin\frac{\alpha_1+\gamma_1}{2}\,, \\ b_0 &= \cos\frac{\beta_2}{2}\cos\frac{\alpha_2+\gamma_2}{2}\,, & b_1 &= \sin\frac{\beta_2}{2}\cos\frac{\gamma_2-\alpha_2}{2}\,, \\ b_2 &= \sin\frac{\beta_2}{2}\sin\frac{\gamma_2-\alpha_2}{2}\,, & b_3 &= \cos\frac{\beta_2}{2}\sin\frac{\alpha_2+\gamma_2}{2}\,, \\ \alpha_3 &= \tan^{-1}\frac{c_1c_3 - c_2c_0}{c_1c_0 + c_2c_3}\,, & \beta_3 &= 2\sin^{-1}\sqrt{c_1^2+c_2^2}\,, \\ \gamma_3 &= \tan^{-1}\frac{c_1c_3 + c_2c_0}{c_1c_0 - c_2c_3}\,. \end{aligned} \tag{6-3, 6-4}$$

From (6-2a) one obtains the combination law for the SU_2 group parameters

$$\begin{aligned} c_0 &= a_0b_0 - a_1b_1 - a_2b_2 - a_3b_3\,, & c_1 &= a_0b_1 + a_1b_0 + a_2b_3 - a_3b_2\,, \\ c_2 &= a_0b_2 - a_1b_3 + a_2b_0 + a_3b_1\,, & c_3 &= a_0b_3 + a_1b_2 - a_2b_1 + a_3b_0\,. \end{aligned} \tag{6-2b}$$

According to (5-177b) and (5-176)

$$-X_\alpha = \left(\frac{\partial\alpha_3}{\partial\alpha_2}\right)_0 \frac{\partial}{\partial\alpha} + \left(\frac{\partial\beta_3}{\partial\alpha_2}\right)_0 \frac{\partial}{\partial\beta} + \left(\frac{\partial\gamma_3}{\partial\alpha_2}\right)_0 \frac{\partial}{\partial\gamma}\,, \tag{6-5a}$$

$$-X_\beta = \left(\frac{\partial\alpha_3}{\partial\beta_2}\right)_0 \frac{\partial}{\partial\alpha} + \left(\frac{\partial\beta_3}{\partial\beta_2}\right)_0 \frac{\partial}{\partial\beta} + \left(\frac{\partial\gamma_3}{\partial\beta_2}\right)_0 \frac{\partial}{\partial\gamma}\,, \tag{6-5b}$$

$$-X_\gamma = \left(\frac{\partial\alpha_3}{\partial\gamma_2}\right)_0 \frac{\partial}{\partial\alpha} + \left(\frac{\partial\beta_3}{\partial\gamma_2}\right)_0 \frac{\partial}{\partial\beta} + \left(\frac{\partial\gamma_3}{\partial\gamma_2}\right)_0 \frac{\partial}{\partial\gamma}\,, \tag{6-5c}$$

where the subscript "0" indicates that the values are to be evaluated at $\alpha_2 = \beta_2 = \gamma_2 = 0$. Using

$$\frac{\partial\alpha_3}{\partial\alpha_2} = \sum_{ij} \frac{\partial\alpha_3}{\partial c_i}\frac{\partial c_i}{\partial b_j}\frac{\partial b_j}{\partial\alpha_2}$$

and similar, as well as (6-2) and (6-5), we can find the differential operators for X_α, X_β and X_γ. With the aid of

$$\alpha X_\alpha = -i\alpha J_z, \quad \beta X_\beta = -i\beta J_y, \quad \gamma X_\gamma = -i\gamma J_z\,,$$

we obtain

$$J_z = \frac{1}{i}\frac{\partial}{\partial\alpha}\,, \tag{6-6a}$$

$$J_y = \frac{1}{i}\left(-\sin\alpha\cot\beta\frac{\partial}{\partial\alpha} + \cos\alpha\frac{\partial}{\partial\beta} + \frac{\sin\alpha}{\sin\beta}\frac{\partial}{\partial\gamma}\right)\,. \tag{6-6b}$$

We can only get two differential operators J_y and J_z from (6-5a), since both X_α and X_γ correspond to the same J_z. The third operator can be found by using the commutator relation $[J_y, J_z] = iJ_x$,

$$J_x = \frac{1}{i}\left(-\cos\alpha\cot\beta\frac{\partial}{\partial\alpha} - \sin\alpha\frac{\partial}{\partial\beta} + \frac{\cos\alpha}{\sin\beta}\frac{\partial}{\partial\gamma}\right) . \tag{6-6c}$$

Equations (6-6) give the infinitesimal operators of the first parameter group, and are identical to Eq. (39) of Eisenberg (1970, p. 98). Therefore the infinitesimal operators of the first parameter group of SO_3 are precisely the well known differential forms of the angular momentum operators J_x, J_y and J_z in the group parameter space.

Similarly, the differential operators of the generators of the intrinsic group $\overline{SO}_3$ can be found using (5-234). Because of the anti-isomorphism between the groups $\overline{SO}_3$ and SO_3, it is known that, corresponding to the SO_3 group element (5-64), the group element of $\overline{SO}_3$ is

$$\overline{R}(\alpha\beta\gamma) = e^{-i\gamma\overline{J}_z}e^{-i\beta\overline{J}_y}e^{-i\alpha\overline{J}_z} . \tag{6-7}$$

The counterpart of (6-5) is

$$\begin{aligned} -\overline{X}_\alpha &= \left(\frac{\partial\alpha_3}{\partial\alpha_1}\right)_0\frac{\partial}{\partial\alpha} + \left(\frac{\partial\beta_3}{\partial\alpha_1}\right)_0\frac{\partial}{\partial\beta} + \left(\frac{\partial\gamma_3}{\partial\alpha_1}\right)_0\frac{\partial}{\partial\gamma} , \\ \left(\frac{\partial\alpha_3}{\partial\alpha_1}\right) &= \sum_{i,j}\frac{\partial\alpha_3}{\partial c_i}\frac{\partial c_i}{\partial a_j}\frac{\partial a_j}{\partial\alpha_1} , \\ &\cdots\cdots\cdots \end{aligned} \tag{6-8}$$

where the subscript "0" means that the values are to be evaluated at $\alpha_1 = \beta_1 = \gamma_1 = 0$. We finally obtain

$$\begin{aligned} \overline{J}_x &= \frac{1}{i}\left(\cos\gamma\cot\beta\frac{\partial}{\partial\gamma} + \sin\gamma\frac{\partial}{\partial\beta} - \frac{\cos\gamma}{\sin\beta}\frac{\partial}{\partial\alpha}\right) = -J_x(\alpha\leftrightarrow\gamma) , \\ \overline{J}_y &= \frac{1}{i}\left(-\sin\gamma\cot\beta\frac{\partial}{\partial\gamma} + \cos\gamma\frac{\partial}{\partial\beta} + \frac{\sin\gamma}{\sin\beta}\frac{\partial}{\partial\alpha}\right) = J_y(\alpha\leftrightarrow\gamma) , \\ \overline{J}_z &= \frac{1}{i}\frac{\partial}{\partial\gamma} = J_z(\alpha\leftrightarrow\gamma) . \end{aligned} \tag{6-9}$$

This is identical with Eq. (29) in Eisenberg (1970, p. 96).

One can verify that the operators in (6-6) and (6-9) satisfy (5-35) or (5-228a), namely,

$$\begin{pmatrix}\overline{J}_x\\ \overline{J}_y\\ \overline{J}_z\end{pmatrix} = \tilde{\mathcal{D}}(\alpha,\beta,\gamma)\begin{pmatrix}J_x\\ J_y\\ J_z\end{pmatrix} , \tag{6-10}$$

where $\tilde{\mathcal{D}}$ is the transpose of the matrix $\mathcal{D}(\alpha\beta\gamma)$ of the adjoint representation ($J = 1$) of SO_3 (see (5-34)).

Comparing (6-10) with (5-35), we find that the infinitesimal operators $\overline{J}_{x,y,z}$ of the intrinsic group $\overline{SO}_3$ are the components $J_{1,2,3}$ of angular momentum in the intrinsic frame. We thus conclude that the projections $J_{1,2,3}$ of angular momentum in the intrinsic frame are the generators of the intrinsic rotation group $\overline{SO}_3$, just as the projections $J_{x,y,z}$ of angular momentum in the fixed frame constitute the generators of SO_3.

Our name for $\overline{G}$, intrinsic group, and the interpretation given in Sec. 5.15 for the generators $\overline{X}_\rho$ of $\overline{G}$, originated from the SO_3 case.

Using (6-6) and (6-9), we can easily check (5-236), that is, the CSCO-I of SO_3 and $\overline{SO}_3$ are equal:

$$J_x^2 + J_y^2 + J_z^2 = \overline{J}_x^2 + \overline{J}_y^2 + \overline{J}_z^2 .$$

Louck (1976, 1970, 1965) studied the transformation between the laboratory (fixed) frame and the intrinsic frame. Louck (1970) and Biedenharn (1968) extended this kind of study to unitary groups.

6.2. Irreps of the Group SO_2

The group SO_2 is Abelian, with elements $R(\varphi) = e^{-i\varphi J_z}$. Each element is a class by itself so the class operators $C(\varphi)$ are still $e^{-i\varphi J_z}$. The generator of SO_2 is J_z. Since SO_2 is a Lie group of rank one, its CSCO-I consists of a single invariant. Obviously, J_z is the CSCO-I of SO_2.

The CSCO-I of a finite group consists of few class operators, while the CSCO-I of a Lie group of rank l consists of l invariants $\{I_i(X_\rho) : i = 1, 2, \ldots, l\}$. The following question may now be raised: What is the relation between the two? For finite groups we proved that all the class operators of a group G must be a CSCO-I of G. The extension of this result to Lie groups implies that all the class operators (the number of which is infinite) of a Lie group must form a CSCO-I of the Lie group. For instance, the infinite number of class operators

$$C(\varphi) = e^{-iJ_z\varphi}, \quad 0 \le \varphi \le 2\pi , \tag{6-11}$$

of the group SO_2 form a CSCO-I of SO_2. On the other hand we know that the properties of a Lie group are determined by the behavior of those elements which lie in the neighborhood of the identity. Therefore, to form a CSCO-I of a Lie group, one merely needs to take the class operators in the neighborhood of the identity.

Expanding the class operator $C(\varphi)$ in (6-11) around $\varphi = 0$, one gets

$$C(\varphi) = 1 - i\varphi J_z + \ldots . \tag{6-12}$$

A simple relation is thus revealed between the CSCO-I $C(\varphi)$ of SO_2 borrowed from the finite group rep theory and the CSCO-I J_z of SO_2 obtained from the Lie group rep theory: By taking the Taylor expansion of the former in the neighborhood of the identity, one can obtain the latter. For the Abelian group SO_2, the CSCO-I J_z is also the CSCO-III. According to Theorem VII in Sec. 3.21, the eigenfunction of J_z in the group parameter space is the complex conjugate of the irreducible matrix element (or character) of SO_2. From (5-177c), we know that $J_z = -i\frac{\partial}{\partial\varphi}$. So the character $\chi^{(m)}(\varphi)$ of SO_2 satisfies the eigenequation

$$-i\frac{\partial}{\partial\varphi}\chi^{(m)}(\varphi)^* = m\chi^{(m)}(\varphi)^* . \tag{6-13}$$

The following two cases are to be considered separately.

1. SO_2. Since $\varphi = 0$ and 2π correspond to the same point in the group parameter space, $\chi^{(m)}(\varphi)$ has to obey the periodicity condition

$$\chi^{(m)}(\varphi = 0) = \chi^{(m)}(\varphi = 2\pi) . \tag{6-14}$$

With the condition (6-14), the eigenfunctions in (6-13) are

$$\chi^{(m)}(\varphi) = e^{-im\varphi}, \quad m = 0, \pm 1, \pm 2, \ldots . \tag{6-15}$$

Clearly, the eigenfunctions $\chi^{(m)}(\varphi)$ form a complete set of orthogonal functions in the interval $(0,2\pi)$ with the weight function

$$\rho(\varphi) = 1 . \tag{6-16}$$

The group volume of SO_2 is

$$g = \int_o^{2\pi} d\varphi = 2\pi \ . \tag{6-17}$$

Consequently the *orthonormality and completeness relations* in (5-247) become

$$\frac{1}{2\pi}\int_0^{2\pi} \chi^{(m)}(\varphi)^* \chi^{(m')}(\varphi) d\varphi = \delta_{mm'} \ , \tag{6-18}$$

$$\frac{1}{2\pi}\sum_{m=0,\pm 1,\ldots} \chi^{(m)}(\varphi) * \chi^{(m)}(\varphi') = \delta(\varphi - \varphi') \ , \tag{6-19}$$

and the projection operator (5-245a) is

$$P^{(m)} = \frac{1}{2\pi}\int_0^{2\pi} e^{-i(J_z - m)\varphi} d\varphi \ . \tag{6-20}$$

2. The double group $SO_2^\dagger$. According to (6-1b), $\varphi = 0$ and $\varphi = 4\pi$ now correspond to the same group element, while $\varphi = 0$ and $\varphi = 2\pi$ do not. The boundary condition (6-14) is replaced by

$$\chi^{(m)}(\varphi = 0) = \chi^{(m)}(\varphi = 4\pi) \ . \tag{6-21}$$

The eigenfunctions in (6-21) are still $\chi^{(m)}(\varphi) = e^{-im\varphi}$, however m now takes half–integer values as well as integer values

$$\chi^{(m)}(\varphi) = e^{-im\varphi} \ , \quad m = 0, \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, \ldots \ . \tag{6-22}$$

The half–integer rep is called the spinor or double–valued rep of SO_2. The weight function is the same as before, $\rho(\varphi) = 1$, but the group volume becomes $g = 4\pi$. The orthonormality and completeness become

$$\begin{aligned} &\frac{1}{4\pi}\int_0^{4\pi} \chi^{(m)}(\varphi)^* \chi^{(m')}(\varphi) d\varphi = \delta_{mm'} \ , \\ &\frac{1}{4\pi}\sum_{m=0,\pm\frac{1}{2},\pm 1,\ldots} \chi^{(m)}(\varphi)^* \chi^{(m)}(\varphi') = \delta(\varphi - \varphi') \ . \end{aligned} \tag{6-23}$$

The projection operator is

$$P^{(m)} = \frac{1}{4\pi}\int_0^{4\pi} e^{-i(J_z - m)\varphi} d\varphi \ . \tag{6-24}$$

6.3. The CSCO–I and Characters of SO_3

In Chapter 5 it was shown that the CSCO–I of SO_3 is $\mathbf{J}^2$. We now proceed to investigate the relationship between $\mathbf{J}^2$ and the class operators of SO_3.

According to Sec. 1.5 all rotations through the same angle φ, about any axes $\mathbf{n}(\theta', \varphi')$, belong to the same class. The rotation operators can be written as

$$R_{\mathbf{n}(\theta'\varphi')}(\varphi) = e^{-i(\mathbf{n}\cdot\mathbf{J})\varphi} \ , \quad 0 \le \theta' \le \pi \ , 0 \le \varphi' \le 2\pi \ , 0 \le \varphi \le \pi \ . \tag{6-25}$$

Using (5-196), we obtain the class operators of SO_3,

$$C(\varphi) = \int_0^{2\pi} d\varphi' \int_0^{\pi} \sin\theta' d\theta' e^{-i(\mathbf{n}\cdot\mathbf{J})\varphi} \ . \tag{6-26}$$

Since J_x, J_y, J_z do not commute with one another, it is not an easy task to perform the integration. Using the coherent state technique and the integration within ordered normal product technique Fan and Ren (1988) was able to find the explicit expression of $C(\varphi)$. Here we will use a short cut to get the same expression. Let $C^{(j)}(\varphi)$ be the eigenvalue of the class operator $C(\varphi)$ in the irrep j. The eigenvalue is independent of the magnetic quantum number m, since the class operator $C(\varphi)$ is an invariant of SO_3. Taking the expectation value of (6-26) in the state $|jm\rangle$ and summing over m we have

$$\sum_m \langle jm|C(\varphi)|jm\rangle = \int_0^{2\pi} d\varphi' \int_0^{\pi} \sin\theta' d\theta' \sum_m \langle jm|e^{-i(\mathbf{n}\cdot\mathbf{J})\varphi}|jm\rangle ,$$

$$(2j+1)C^{(j)}(\varphi) = 4\pi\chi^{(j)}(\varphi) , \tag{6-27a}$$

where $\chi^{(j)}(\varphi)$ is the character of SO_3, and will be calculated easily in a moment. Using the expression for the character $\chi(\varphi)^{(j)}$ in (6-64) and replacing the eigenvalue $2j+1$ by the operator $\hat{t} = \sqrt{4\mathbf{J}^2+1}$ we get the class operator

$$C(\varphi) = 4\pi \frac{\sin(\frac{1}{2}\hat{t}\varphi)}{\hat{t}\sin(\frac{\varphi}{2})} , \tag{6-27b}$$

which is exactly the same as Eq. (30) in Fan & Ren (1988). Once again we have a simple relation between the CSCO-I $C(\varphi)$ of SO_3 extrapolated from the finite group rep theory and the CSCO-I $\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2$ of SO_3 obtained from the Lie group rep theory.

For small φ, we have the following expansion

$$C(\varphi) = 4\pi\Big[1 - \frac{1}{3!}\mathbf{J}^2\varphi^2 + \frac{1}{5!}\mathbf{J}^2(\mathbf{J}^2 - \tfrac{1}{3})\varphi^4 + \ldots\Big] . \tag{6-27c}$$

According to (5-197), the volume of the elements belonging to the class φ is

$$g(\varphi) = \int_0^{2\pi} d\varphi' \int_0^{\pi} \sin\theta' d\theta' = 4\pi . \tag{6-28}$$

One sees that $g(\varphi)$ is independent of φ.

To find the characters and the density function in the class parameter space, we have to know the differential operator of $\mathbf{J}^2$ in the class parameter space. Let us first find the infinitesimal operators of the first parameter group of SO_3 with $(\theta', \varphi', \varphi)$ as the group parameters. In analogy with (6-1), we consider the product of two successive rotations

$$R(\theta_3'\varphi_3'\varphi_3) = R(\theta_2'\varphi_2'\varphi_2)R(\theta_1'\varphi_1'\varphi_1) . \tag{6-29}$$

The combination law for the parameters $(\theta', \varphi', \varphi)$ is still not easy to write out explicitly, and is again obtained implicitly through the parameters (6-2a) of the group SU_2. The relations between these two sets of parameters are given by Smirnov (1951).

$$\begin{aligned} a_0 &= \cos(\varphi_1/2) , & a_1 &= \sin\theta_1' \cos\varphi_1' \sin(\varphi_1/2) , \\ a_2 &= \sin\theta_1' \sin\varphi_1' \sin(\varphi_1/2) , & a_2 &= \cos\theta_1' \sin(\varphi_1/2) . \end{aligned} \tag{6-30}$$

As in (6-5a), we have

$$-X_\varphi = \left(\frac{\partial\theta_3'}{\partial\varphi_2}\right)_0 \frac{\partial}{\partial\theta'} + \left(\frac{\partial\varphi_3'}{\partial\varphi_2}\right)_0 \frac{\partial}{\partial\varphi'} + \left(\frac{\partial\varphi_3}{\partial\varphi_2}\right)_0 \frac{\partial}{\partial\varphi} , \tag{6-31}$$

where the subscript "0" means evaluate at $\varphi_2 = 0$. It can be shown that the infinitesimal operators $X_{\theta'}$ and $X_{\varphi'}$ corresponding to the parameters θ' and φ' are zero. Using

$$\left(\frac{\partial\theta_3'}{\partial\varphi_2}\right)_0 = \left(\frac{\partial\theta_3'}{\partial c_i}\right)_0 \frac{\partial c_i}{\partial b_j}\left(\frac{\partial b_j}{\partial\varphi_2}\right)_0 ,$$
$$\cdots\cdots\cdots \tag{6-32}$$

as well as (6-2b) and (6-30), we can find the operator X_φ. From $\exp(\varphi X_\varphi) = \exp[-i(\mathbf{J}\cdot\mathbf{n})\varphi]$ we get

$$X_\varphi = -i(\sin\theta'\cos\varphi' J_x + \sin\theta'\sin\varphi' J_y + \cos\theta' J_z) . \tag{6-33}$$

Comparing (6-31) with (6-33) we finally have

$$\begin{aligned}
J_x &= \frac{1}{i}\left[\sin\theta'\cos\varphi'\frac{\partial}{\partial\varphi} + \frac{1}{2}\left(\sin\varphi' + \cos\theta'\cos\varphi'\cot\frac{\varphi}{2}\right)\frac{\partial}{\partial\theta'}\right.\\
&\quad \left. + \frac{\cos\theta'\cos\varphi'\sin(\frac{\varphi}{2}) - \sin\varphi'\cos(\frac{\varphi}{2})}{2\sin\theta'\sin(\frac{\varphi}{2})}\frac{\partial}{\partial\varphi'}\right] ,\\
J_y &= \frac{1}{i}\left[\sin\theta'\sin\varphi'\frac{\partial}{\partial\varphi} + \frac{1}{2}\left(-\cos\varphi' + \cos\theta'\sin\varphi'\cot\frac{\varphi}{2}\right)\frac{\partial}{\partial\theta'}\right.\\
&\quad \left. + \frac{\cos\theta'\sin\varphi'\sin(\frac{\varphi}{2}) + \cos\varphi'\cos(\frac{\varphi}{2})}{2\sin\theta'\sin(\frac{\varphi}{2})}\frac{\partial}{\partial\varphi'}\right] ,\\
J_z &= \frac{1}{i}\left[\cos\theta'\frac{\partial}{\partial\varphi} - \frac{1}{2}\sin\theta'\cot(\tfrac{\varphi}{2})\frac{\partial}{\partial\theta'} - \frac{1}{2}\frac{\partial}{\partial\varphi'}\right] ,\\
J^2 &= -\frac{1}{\sin^2(\frac{\varphi}{2})}\frac{\partial}{\partial\varphi}\left(\sin^2\frac{\varphi}{2}\frac{\partial}{\partial\varphi}\right) - \frac{1}{4\sin^2(\frac{\varphi}{2})\sin\theta'}\frac{\partial}{\partial\theta'}\left(\sin\theta'\frac{\partial}{\partial\theta'}\right)\\
&\quad - \frac{1}{4\sin^2(\frac{\varphi}{2})\sin^2\theta'}\frac{\partial^2}{\partial\varphi'^2} .
\end{aligned} \tag{6-34}$$

According to Theorem II in Sec. 3.21, the character $\chi^{(\nu)}(\varphi)$ of SO_3 satisfies the eigenfunction

$$J^2\chi^{(\nu)}(\varphi) = \nu\chi^{(\nu)}(\varphi) , \tag{6-35a}$$

that is,

$$-\frac{1}{\sin^2(\frac{\varphi}{2})}\frac{\partial}{\partial\varphi}\left(\sin^2\frac{\varphi}{2}\frac{\partial}{\partial\varphi}\right)\chi^{(\nu)}(\varphi) = \nu\chi^{(\nu)}(\varphi) , \tag{6-35b}$$

or expressed differently

$$-\frac{1}{\rho(\varphi)}\frac{d}{d\varphi}\left(\rho(\varphi)\frac{d}{d\varphi}\right)\chi^{(\nu)}(\varphi) = \nu\chi^{(\nu)}(\varphi) , \tag{6-35c}$$

$$\rho(\varphi) = 4\sin^2(\tfrac{\varphi}{2}) = 2(1-\cos\varphi) . \tag{6-36}$$

We will see that $\rho(\varphi)$ is the density function in class parameter space. The factor 4 in front of $\sin^2(\frac{\varphi}{2})$ is introduced so that the density function is the same as that used by Hamermesh (1962).[1)]

From (6-36) and (5-201), the group volume of SO_3 is

$$g = \int_0^\pi \rho(\varphi)d\varphi \int_0^{2\pi} d\varphi' \int_0^\pi \sin\theta' d\theta' = 8\pi^2 . \tag{6-37}$$

[1)]The density function can be enlarged or reduced by any constant factor without affecting the ratios $\rho(\varphi)/g$ and $\rho(a)/g$, and therefore without affecting the final results.

Let

$$u^{(\nu)}(\varphi) = \sin\tfrac{\varphi}{2}\chi^{(\nu)}(\varphi)\ . \tag{6-38}$$

Equation (6-35b) becomes

$$\frac{d^2u^{(\nu)}(\varphi)}{d^2\varphi} = -\left(j+\tfrac{1}{2}\right)^2 u^{(\nu)}(\varphi)\ ,$$
$$\left(j+\tfrac{1}{2}\right)^2 = \nu+\tfrac{1}{4},\quad \nu = j(j+1)\ . \tag{6-39}$$

The solution is $u^{(\nu)}(\varphi) \equiv u^{(j)}(\varphi) = \sin(j+\frac{1}{2})\varphi$. Another solution $\cos(j+\frac{1}{2})\varphi$ is discarded, since $\chi^{(\nu)}(\varphi) = \cos(j+\frac{1}{2})\varphi/\sin\frac{\varphi}{2}$ diverges at $\varphi = 0$. The eigenvalues j are to be determined from the boundary conditions.

From (6-35c) and making use of Greens theorem,

$$\rho(\varphi)\left(\chi^{(j')}\frac{d\chi^{(j)}}{d\varphi} - \chi^{(j)}\frac{d\chi^{(j')}}{d\varphi}\right)\Bigg|_a^b = [j(j+1) - j'(j'+1)]\int_a^b \chi^{(j')}\chi^{(j)}\rho(\varphi)d\varphi\ , \tag{6-40}$$

$$\chi^{(j)}(\varphi) = \frac{\sin(j+\frac{1}{2})\varphi}{\sin(\frac{\varphi}{2})}\ . \tag{6-41}$$

If $\chi^{(j)}$ or $\frac{d\chi^{(j)}}{d\varphi}$ vanishes at the boundaries $\varphi = a$ and $\varphi = b$, it follows from (6-40) that the functions $\chi^{(j)}$ form an orthogonal complete set in the interval $[a,b]$ with the weight $\rho(\varphi)$,

$$\int_a^b \chi^{(j)}(\varphi)\chi^{(j')}(\varphi)\rho(\varphi)d\varphi = 0,\quad \text{for } j \neq j'\ . \tag{6-42}$$

Equation (6-41) does not vanish at $\varphi = 0, \pi$, or 2π; therefore the boundary condition has to be chosen as

$$\frac{d\chi^{(j)}(\varphi)}{d\varphi} = 0,\quad \text{for } \varphi = a, b\ . \tag{6-43a}$$

From (6-41) we obtain

$$\frac{d\chi^{(j)}(\varphi)}{d\varphi} = \frac{\left(j+\frac{1}{2}\right)\cos\left(j+\frac{1}{2}\right)\varphi\sin\frac{\varphi}{2} - \frac{1}{2}\sin\left(j+\frac{1}{2}\right)\varphi\cos\frac{\varphi}{2}}{\sin^2\frac{\varphi}{2}}\ . \tag{6-43'}$$

Using L'Hopitals rule we find its extrema at $\varphi = 0$ or 2π, that is,

$$\left.\frac{d\chi^{(j)}(\varphi)}{d\varphi}\right|_{\varphi=0 \text{ or } 2\pi} = -j(j+1)\left.\frac{\sin\left(j+\frac{1}{2}\right)\varphi}{\cos\frac{\varphi}{2}}\right|_{\varphi=0 \text{ or } 2\pi}\ . \tag{6-43b}$$

Using the L'Hopital rule again, we get its extremum at $\varphi = \pi$

$$\left.\frac{d\chi^{(j)}(\varphi)}{d\varphi}\right|_{\varphi=\pi} = (2j+1)j(j+1)\left.\frac{\cos\left(j+\frac{1}{2}\right)\varphi}{\sin\frac{\varphi}{2}}\right|_{\varphi=\pi}\ . \tag{6-43c}$$

The boundary a for φ is always chosen to be zero, while the boundary b may be chosen as π or 2π depending on whether the group being considered is SO_3 or $SO_3^\dagger$.

1. The case of SO_3. The range of φ is specified by (6-25), that is, $a = 0$ and $b = \pi$. It follows from (6-43b) and (6-43c) that the quantum number j are necessarily integers, $j = 0, 1, 2, \ldots$. Therefore $\chi^{(j)}(\varphi)$ form an orthogonal complete set of functions in the interval $[0,\pi]$. Putting in the norm we have

$$\frac{1}{2\pi}\int_0^\pi \chi^{(j)}(\varphi)\chi^{(j')}(\varphi)\rho(\varphi)d\varphi = \delta_{jj'},\quad j,j' = 0,1,2,\ldots\ . \tag{6-44a}$$

$$\frac{1}{2\pi}\sum_{j=0,1,2,\ldots}\chi^{(j)}(\varphi)\chi^{(j)}(\varphi')\rho(\varphi)=\delta(\varphi-\varphi')\ . \tag{6-44b}$$

This is the realization of (5-244) for the group SO_3. Now $g=8\pi^2$ and $g(\varphi)=4\pi$.

It is seen that the weight function (6-36) in the differential equation (6-35b) is just the density function and (6-41) is the irreducible character of SO_3.

The purpose of using this awkward way to find the character of SO_3 is to show the applicability of the theorems for the finite groups to the Lie groups. Later in Eq. (6-64) we will give a very simple way to determine the character of SO_3.

2. The case of $SO_3^\dagger$. For the double group $SO_3^\dagger$, (6-1d), the range of φ is from zero to 2π. Therefore the boundaries in (6-43b) become $a=0$ and $b=2\pi$. From (6-43b) we obtain $j=0,\frac{1}{2},1,\frac{3}{2},\ldots$. The functions $\chi^{(j)}(\varphi)$ of (6-41) form an *orthogonal complete set* in the interval $[0,2\pi]$:

$$\frac{1}{4\pi}\int_0^{2\pi}\chi^{(j)}(\varphi)\chi^{(j')}(\varphi)\rho(\varphi)d\varphi=\delta_{jj'},\quad j,j'=0,\tfrac{1}{2},1,\tfrac{3}{2}\ ,\ldots \tag{6-45a}$$

$$\frac{1}{4\pi}\sum_{j=0,\frac{1}{2},1,\frac{3}{2},\ldots}\chi^{(j)}(\varphi)\chi^{(j)}(\varphi')\rho(\varphi)=\delta(\varphi-\varphi')\ . \tag{6-45b}$$

For integer j, (6-45) goes back to (6-44).

Remark: The orthonormality (6-44a) remains true when both j and j' are half-integers, but is not true when j is an integer and j' is a half-integer. To restore the orthogonal property for the latter case, one has to extend the interval of φ from $[0,\pi]$ to $[0,2\pi]$ so (6-44a) is replaced by (6-45a).

Setting $\varphi=0$ in (6-41), we obtain the character of the identity, that is, the dimension of the irrep j of SO_3,

$$h_\nu=h_j=2j+1\ .$$

From (5-242) we obtain the projection operators for the groups SO_3 and $SO_3^\dagger$:

$$SO_3:\ P^{(j)}=\frac{2j+1}{2\pi^2}\int_0^{\pi}\sin\left(j+\tfrac{1}{2}\right)\varphi\ \sin\tfrac{\varphi}{2}C(\varphi)d\varphi,\quad j=0,1,2,\ldots \tag{6-46a}$$

$$SO_3^\dagger:\ P^{(j)}=\frac{2j+1}{4\pi^2}\int_0^{2\pi}\sin\left(j+\tfrac{1}{2}\right)\varphi\ \sin\tfrac{\varphi}{2}C(\varphi)d\varphi,\quad j=0,\tfrac{1}{2},1,\tfrac{3}{2}\ ,\ldots \tag{6-46b}$$

6.4. The CSCO-III and Irreducible Matrix Elements of SO_3

We now return to the group-parameter space. SO_3 is a Lie group with three parameters. The CSCO-III should consist of three operators. In addition to $\mathbf{J}^2$, we need two other operators.

We choose the group chain $SO_3\supset SO_2$ to classify the irreducible basis of SO_3. The corresponding intrinsic group chain is $S\overline{O}_3\supset S\overline{O}_2$. J_z and $\overline{J}_z$ are the CSCO-I of SO_2 and $\overline{SO}_2$, respectively. Let

$$K=(C,C(s),\overline{C}(s))=(\mathbf{J}^2,J_z,\overline{J}_z)\ .$$

K is the CSCO-III of SO_3.

Choosing the Euler angles as the group parameters, we have from (6-6) and (6-9) the following differential operators,

$$J^2=-\frac{1}{\sin\beta}\frac{\partial}{\partial\beta}\left(\sin\beta\frac{\partial}{\partial\beta}\right)-\frac{1}{\sin^2\beta}\left(\frac{\partial^2}{\partial\alpha^2}+\frac{\partial^2}{\partial\gamma^2}\right)+\frac{2\cos\beta}{\sin^2\beta}\frac{\partial^2}{\partial\alpha\partial\gamma}\ , \tag{6-47a}$$

$$J_z = \frac{1}{i}\frac{\partial}{\partial\alpha}, \quad \overline{J}_z = \frac{1}{i}\frac{\partial}{\partial\gamma} . \tag{6-47b}$$

The simultaneous eigenfunctions of $\mathbf{J}^2, J_z$ and $\overline{J}_z$ are the complex conjugate of the well known D–functions (Rose 1957)

$$\begin{pmatrix} \mathbf{J}^2 \\ J_z \\ \overline{J}_z \end{pmatrix} D^{(j)*}_{mk}(\alpha\beta\gamma) = \begin{pmatrix} j(j+1) \\ m \\ k \end{pmatrix} D^{(j)*}_{mk}(\alpha\beta\gamma) . \tag{6-48}$$

For a given set of quantum numbers (j, m, k), there is only one solution $D^{(j)*}_{mk}(\alpha\beta\gamma)$. Equation (6-48) can be treated by the separation of variables method:

$$D^{(j)*}_{mk}(\alpha\beta\gamma) = e^{im\alpha} d^{(j)}_{mk}(\beta) e^{ik\gamma} , \tag{6-49}$$

$$\left[-\frac{d}{d\beta}\sin\beta\frac{d}{d\beta} + \frac{1}{\sin\beta}(m^2 + k^2 - 2mk\cos\beta)\right] d^{(j)}_{mk}(\beta) = j(j+1)\sin\beta d^{(j)}_{mk}(\beta) . \tag{6-50}$$

The density or weight function $\rho(\alpha\beta\gamma)$ can also be factorized, $\rho(\alpha\beta\gamma) = \rho(\alpha)\rho(\beta)\rho(\gamma)$. Comparing (6-47b) with (6-13), we see that $\rho(\alpha) = \rho(\gamma) = 1$. Comparing (6-50) with (6-35c), we have $\rho(\beta) = \sin\beta$. Therefore

$$\rho(\alpha\beta\gamma) = \sin\beta . \tag{6-51}$$

1. The case of SO_3. From (6-1c), the group volume is

$$g = \int_0^{2\pi} d\alpha \int_0^{2\pi} d\gamma \int_0^{\pi} \sin\beta d\beta = 8\pi^2 ,$$

in agreement with (6-37). The eigenfunctions

$$\psi^{(j)k}_m(\alpha\beta\gamma) = \sqrt{\frac{2j+1}{8\pi^2}} D^{(j)*}_{mk}(\alpha\beta\gamma), \quad j = 0, 1, 2, 3, \ldots \tag{6-52}$$

of the CSCO–III form an orthonormal set of functions over the intervals $[0, 2\pi]$ for α and γ, and $[0, \pi]$ for β, with the weight $\rho(\beta) = \sin\beta$,

$$\int_0^{2\pi} d\alpha \int_0^{2\pi} d\gamma \int_0^{\pi} \sin\beta d\beta \psi^{(j)k}_m(\alpha\beta\gamma)^* \psi^{(j')k'}_{m'}(\alpha\beta\gamma) = \delta_{jj'}\delta_{mm'}\delta_{kk'} , \tag{6-53a}$$

$$\sum_{j=0,1,2,\ldots} \sum_{m=-j}^{j} \sum_{k=-j}^{j} \psi^{(j)k}_m(\alpha\beta\gamma)^* \psi^{(j)k}_m(\alpha\beta\gamma)\sin\beta = \delta(\alpha-\alpha')\delta(\beta-\beta')\delta(\gamma-\gamma') . \tag{6-53b}$$

The generalized projection operator $P^{(j)}_{mk}$ of (5-245a) now becomes

$$P^{(j)}_{mk} = \frac{2j+1}{8\pi^2} \int_0^{2\pi} d\alpha \int_0^{2\pi} d\gamma \int_0^{\pi} \sin\beta d\beta D^{(j)*}_{mk}(\alpha\beta\gamma) R(\alpha\beta\gamma) . \tag{6-54}$$

2. The case of $SO_3^{\dagger}$. From (6-1d), the group volume of $SO_3^{\dagger}$ is

$$g = \int_0^{2\pi} d\alpha \int_0^{4\pi} d\gamma \int_0^{\pi} \sin\beta d\beta = 16\pi^2 , \tag{6-55}$$

$$\psi^{(j)k}_m(\alpha\beta\gamma) = \frac{\sqrt{2j+1}}{4\pi} D^{(j)*}_{mk}(\alpha\beta\gamma) \quad j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots \tag{6-56}$$

Those functions form an orthonormal set over the interval $[0,2\pi],[0,\pi]$ and $[0,4\pi]$ for α , β and γ, respectively, with the weight $\sin\beta$,

$$\int_0^{2\pi} d\alpha \int_0^{4\pi} d\gamma \int_0^{\pi} \sin\beta d\beta \psi_m^{(j)k}(\alpha\beta\gamma)^* \psi_{m'}^{(j')k'}(\alpha\beta\gamma) = \delta_{jj'}\delta_{mm'}\delta_{kk'} \ , \tag{6-57a}$$

$$\sum_{j=0,\frac{1}{2},1,\ldots} \sum_m \sum_k \psi_m^{(j)k}(\alpha\beta\gamma)^* \psi_m^{(j)k}(\alpha'\beta'\gamma') \sin\beta = \delta(\alpha-\alpha')\delta(\beta-\beta')\delta(\gamma-\gamma') \ . \tag{6-57b}$$

The projection operator is

$$P_{mk}^{(j)} = \frac{2j+1}{16\pi^2} \int_0^{2\pi} d\alpha \int_0^{4\pi} d\gamma \int_0^{\pi} \sin\beta d\beta D_{mk}^{(j)*}(\alpha\beta\gamma) R(\alpha\beta\gamma) \ . \tag{6-58}$$

The projection operators of (6-54) or (6-58) satisfy the following eigenequation

$$\begin{pmatrix} J^2 \\ J_z \\ \overline{J}_z \end{pmatrix} P_{mk}^{(j)} = \begin{pmatrix} j(j+1) \\ m \\ k \end{pmatrix} P_{mk}^{(j)} \ . \tag{6-59}$$

6.5. The CSCO–II and Irreducible Bases of SO_3

$(\mathbf{J}^2, J_z)$ is the CSCO–II of SO_3, and is the complete set of commuting operators in the (θ,φ) space. The differential operators of $\mathbf{J}^2$ and J_z in the (θ,φ) space are well known in quantum mechanics as

$$J^2 = -\frac{1}{\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin\theta}\frac{\partial}{\partial\varphi^2}\right) \ ,$$

$$J_z = \frac{1}{i}\frac{\partial}{\partial\varphi} \ . \tag{6-60}$$

The simultaneous eigenfunctions of the CSCO–II are the spherical harmonic functions $Y_{lm}(\theta,\varphi)$,

$$\begin{pmatrix} J^2 \\ J_z \end{pmatrix} Y_{lm}(\theta,\varphi) = \begin{pmatrix} l(l+1) \\ m \end{pmatrix} Y_{lm}(\theta,\varphi) \ . \tag{6-61}$$

$Y_{lm}(\theta,\varphi)$ form an orthonormal set over the intervals $[0,\pi]$ for θ and $[0,2\pi]$ for φ,

$$\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta Y_{lm}^*(\theta,\varphi) Y_{l'm'}(\theta,\varphi) = \delta_{ll'}\delta_{mm'} \ , \tag{6-62a}$$

$$\sum_{l=0,1,2,\ldots} \sum_m Y_{lm}^*(\theta,\varphi) Y_{lm}(\theta',\varphi') \sin\theta = \delta(\theta-\theta')\delta(\varphi-\varphi') \ . \tag{6-62b}$$

Y_{lm} is the $SO_3 \supset SO_2$ irreducible basis.

Analogously, the $SO_3^\dagger \supset SO_2^\dagger$ (or $SU_2 \supset SO_2$) irreducible basis satisfies the following eigenequations

$$\begin{pmatrix} J^2 \\ J_z \end{pmatrix} \psi_m^{(j)} = \begin{pmatrix} j(j+1) \\ m \end{pmatrix} \psi_m^{(j)} \ . \tag{6-63}$$

Incidentally, we can use the fact that $\psi_m^{(j)}$ is the $SO_3 \supset SO_2$ irreducible basis to calculate the simple characters of SO_3. Since the characters is a function only of class, it suffices to calculate the characters of the rotation $R_z(\varphi)$

$$\begin{aligned} \chi^{(j)}(\varphi) &= \sum_{m=-j}^{j} \langle \psi_m^{(j)} | e^{-iJ_z\varphi} | \psi_m^{(j)} \rangle = \sum_{m=-j}^{j} e^{-im\varphi} \\ &= \left[e^{ij\varphi} + e^{-ij\varphi} + e^{i(j-1)\varphi} + \ldots\right](e^{i\varphi/2} - e^{-i\varphi/2})(e^{i\varphi/2} - e^{-i\varphi/2})^{-1} \\ &= \frac{\sin(j+\frac{1}{2})\varphi}{\sin(\frac{\varphi}{2})} \ , \end{aligned} \tag{6-64}$$

in agreement with (6-41). This is the standard method to calculate the characters of SO_3 or SU_2.

6.6. The Intrinsic State of SO_3

In the case when a given irrep j occurs more than once, we need to introduce the intrinsic quantum numbers to distinguish these equivalent irreps. With this purpose in mind, we first introduce the intrinsic state of SO_3. The definition of the intrinsic state $\Phi_0(X)$ is given by (5-235), that is by

$$\overline{R}(\alpha\beta\gamma)\Phi_0(X) = R(\alpha\beta\gamma)\Phi_0(X) \ . \tag{6-65}$$

To give some physical meaning to the intrinsic state, we shall consider the collective rotation of a deformed nucleus. A Hartree–Fock (HF) state of a nucleus with an open shell is in general not spherical; in most cases it is prolate. The HF states may have different orientations in the space, such as Φ_1 and Φ_{a_0} (see Fig. 6.6-1), where $\Phi_{a_0}(X) = R(a_0)\Phi_1(X)$, or more generally, $\Phi_a(X) = R(a)\Phi_1(X)$ and $R(a)$ is a rotation operator. All these HF states are energy degenerate.

We can define three kinds of coordinate axes: (i) the fixed (external) axes x, y, z, (ii) the symmetry axes x_0, y_0, z_0 of the nucleus, (iii) the intrinsic (body-fixed) axes 1,2,3. From (6-65) it is known that the HF state whose intrinsic axes coincide with the external ones is the intrinsic state. Therefore the choice of the intrinsic state depends on the choice of the intrinsic axes. There are two possible choices.

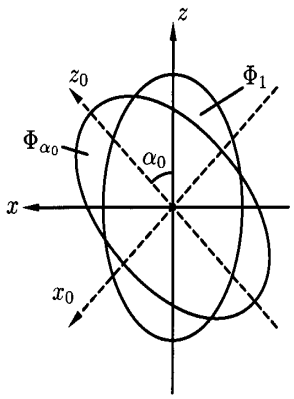
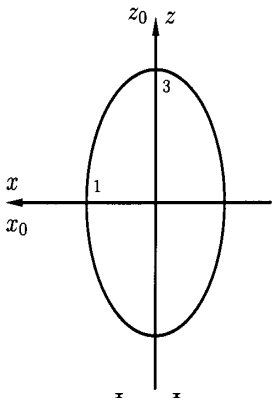
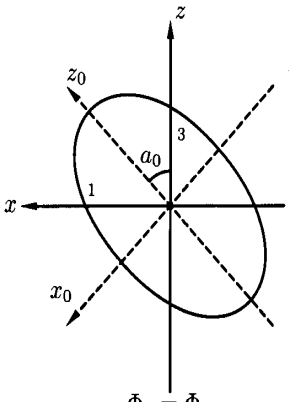


Fig. 6.6-1



$\Phi_0 = \Phi_1$

Fig. 6.6-2



$\Phi_0 = \Phi_{a_0}$

Fig. 6.6-3

1. Choose the symmetric axes of the nucleus as the intrinsic axes. In such a case, the axes (x_0, y_0, z_0) coincide with the axes (1,2,3), and the state Φ_1 (see Fig. 6.6-2) is our intrinsic state.

2. The intrinsic axes (1,2,3) do not coincide with the symmetry axes (x_0, y_0, z_0). Let a_0 be the orientation angle of the axes (x_0, y_0, z_0) with respect to the axes (1,2,3). In this case, the HF state $\Phi_{a_0}(X)$ (see Fig. 6.6-3) is our intrinsic state.

It is thus seen that the arbitrariness in the choice of the intrinsic state stems from the freedom in the choice of the intrinsic axes. In principle any state $\Phi_a(X)$ can be chosen as the intrinsic state. Obviously the first choice is the most convenient one and afterwards we always assume that the symmetry axes of the prolate nucleus are the intrinsic axes and Φ_1 is the intrinsic state. All other HF state $\Phi_a(X)$ can be generated from Φ_0 through the rotation $R(a)$:

$$\Phi_a(X) = R(a)\Phi_0(X) \ . \tag{6-66}$$

Equations (6-65) and (6-66) specify the action of the intrinsic group element on any state $\Phi_a(X)$.

$$\overline{R}(b)\Phi_a(X) = \overline{R}(b)R(a)\Phi_0(X) = R(a)R(b)\Phi_0(X) = R(a)\Phi_b(X) \ .$$

In Elliott's SU_3 model for nuclear rotation (Elliott 1958, see Sec. 9.8), the so–called leading state $\phi((\lambda\mu)\overline{\varepsilon}\overline{\Lambda}\overline{\nu})$ is defined as the intrinsic state with $\overline{\varepsilon} = 2\lambda + \mu, \overline{\Lambda} = \mu/2$ and $\overline{\nu} = \mu$. The physical meaning of Elliott's intrinsic state is identical to that discussed here.

Now the meaning of (6-65) becomes clear: $\overline{R}(\alpha\beta\gamma)$ and $R(\alpha\beta\gamma)$ are rotation operators about the intrinsic and external axes, respectively. They have the same effect on the intrinsic state Φ_0, since Φ_0 is the HF state whose symmetry axes, which have been chosen as the intrinsic axes, coincide with the external ones (see Fig. 6.6-2).

6.7. The Projection State of SO_3

Suppose that a non–spherical HF state has axial symmetry. Although it does not have definite total angular momentum, it has definite $J_z = K$. From (6-65) one has

$$\overline{J}_z\Phi_0^{(K)}(X) = J_z\Phi_0^{(K)}(X) = K\Phi_0^{(K)}(X) \ , \tag{6-67}$$

namely, the z–component of angular momentum of the HF state $\Phi_0(X)$, whose symmetry axes coincide with the external ones, is just the third component of the angular momentum in the intrinsic frame.

Applying the projection operator $P^{(J)}_{MK'}$ on the intrinsic state $\Phi_0^{(K)}(X)$ yields a state with definite angular momentum J and z–component M, if it does not vanish. Now let us study the problem of the intrinsic component of the total angular momentum **J** of the projected state. It was pointed out in Sec. 3.13 that not every element of the intrinsic group has a definite action on the state in the configuration space, but only the class operators of certain intrinsic subgroups have definite actions. The method for finding these class operators is as follows: First find all the operators which leave the intrinsic state $\Phi_0^{(K)}(X)$ unchanged. For instance, for the intrinsic state $\Phi_0^{(K)}(X)$ in (6-67), these operators are seen to be

$$R'_z(\varphi)\Phi_0^{(K)}(X) = \Phi_0^{(K)}(X) \ ,$$

$$R'_z(\varphi) = e^{-i\varphi(J_z - K)} \ . \tag{6-68}$$

This means that $\Phi_0^{(K)}(X)$ is an axially symmetric state.

According to Sec. 3.13, only the intrinsic group elements $\overline{R}_z(\varphi) = e^{-i\overline{J}_z\varphi}$, and thus the operator $\overline{J}_z$ have definite meaning.

From (6-59) one has

$$\overline{J}_z P^{(J)}_{MK'}\Phi_0^{(K)}(X) = (\overline{J}_z P^{(J)}_{MK'})\Phi_0^{(K)}(X) = K' P^{(J)}_{MK'}\Phi_0^{(K)}(X) \ .$$

On the other hand, from (6-67) one has

$$\overline{J}_z P^{(J)}_{MK'}\Phi_0^{(K)}(X) = P^{(J)}_{MK'}\overline{J}_z\Phi_0^{(K)}(X) = K P^{(J)}_{MK'}\Phi_0^{(K)}(X) \ .$$

Comparing the above two equations, one gets

$$P^{(J)}_{MK'}\Phi_0^{(K)}(X) = \delta_{KK'}\Psi_M^{(J)K}(X) \ , \tag{6-69}$$

$$\Psi_M^{(J)K}(X) = \frac{2J+1}{8\pi^2}\int D^{(J)*}_{MK}(\alpha\beta\gamma)R(\alpha\beta\gamma)\Phi_0^{(K)}(X)\sin\beta d\alpha d\beta d\gamma \ . \tag{6-70}$$

Equation (6-69) shows that for an axially symmetric state, the third component of its angular momentum in the intrinsic frame is determined entirely by the z-component of the angular momentum of the intrinsic state. This is precisely the mathematical expression of the well known observation in nuclear physics that the angular momentum of a nucleus along its symmetry axis comes solely from the intrinsic motion of nucleons, in other words a nucleus has no collective rotation about its symmetry axis (Bohr 1975).

According to the above discussion, the projection state $\Psi_M^{(J)K}$ satisfies the simultaneous eigenequations

$$\begin{pmatrix} J^2 \\ J_z \\ \overline{J}_z \end{pmatrix} \Psi_M^{(J)K}(X) = \begin{pmatrix} J(J+1) \\ M \\ K \end{pmatrix} \Psi_M^{(J)K}(X) \ . \tag{6-71}$$

The intrinsic state

$$\Phi\left((\lambda\mu),\ \overline{\varepsilon} = 2\lambda + \mu,\ \overline{\Lambda} = \tfrac{\mu}{2},\ \overline{\nu} = \mu\right) \ ,$$

in Elliott's SU_3 model does not have definite J_z values. The range of J_z is $K = \mu, \mu-2, \ldots, 1$ or 0. Using the projection operator one can likewise pick out the component with given J, M, K from the intrinsic state

$$\Psi_{MK}^{(J)} = P_{MK}^{(J)} \phi((\lambda\mu)\overline{\varepsilon}\overline{\Lambda}\overline{\nu}) \ , \quad K = \mu,\ \mu-2, \ldots, 1 \quad \text{or} \quad 0 \ . \tag{6-72}$$

The intrinsic quantum number K is used to distinguish the different states with the same J and M, which differ in their intrinsic excitation states. The energy levels with the same quantum number K form a rotation band. Therefore the intrinsic quantum numbers K may be used to characterize the rotation bands (Elliott 1958, Arima 1981).

Another point worth mentioning is that the projected states (6-70) are orthogonal with respect to J and M, but not orthogonal with respect to the intrinsic quantum number K. From (5-245b) and (5-245c) one has

$$\left\langle \Psi_{M'}^{(J')K'} | \Psi_M^{(J)K} \right\rangle = \left\langle \Phi_0 | P_{K'M'}^{(J')} P_{MK}^{(J)} \middle| \Phi_0 \right\rangle = \delta_{JJ'}\delta_{MM'} \left\langle \Phi_0 | P_{K'K}^{(J)} | \Phi_0 \right\rangle \ . \tag{6-73}$$

6.8. Irreducible Tensors of SO_3 and $\overline{SO}_3$

6.8.1. The irreducible tensors $T_\rho^{(1)}$ of the adjoint rep of SO_3 and $\overline{SO}_3$

The infinitesimal operators J_x, J_y and J_z of SO_3 form a basis for the adjoint rep of SO_3. As pointed out in Sec. 5.17, when the irreducible matrix elements are given by the solutions of (6-48), in other words, when the $SO_3 \supset SO_2$ irreducible basis is used, only through a suitable linear combination of J_x, J_y and J_z can we obtain the irreducible tensor $T_\rho^{(1)} = J_\rho, \rho = 1, 0, -1$, of the adjoint rep of SO_3,

$$J_1 = -\frac{1}{\sqrt{2}}(J_x + iJ_y) \ , \quad J_0 = J_z \ , \quad J_{-1} = \frac{1}{\sqrt{2}}(J_x - iJ_y) \ . \tag{6-74}$$

Similarly, the irreducible tensor of the adjoint rep of $\overline{SO}_3$ is $\overline{T}^{(1)} = \overline{J}_\rho, \rho = 1, 0, -1$,

$$\overline{J}_1 = -\frac{1}{\sqrt{2}}(\overline{J}_x + i\overline{J}_y) \ , \quad \overline{J}_0 = \overline{J}_z \ , \quad \overline{J}_{-1} = \frac{1}{\sqrt{2}}(\overline{J}_x - i\overline{J}_y) \ . \tag{6-75}$$

From (5-228) one has

$$\overline{J}_\rho = \sum_\sigma D_{\sigma\rho}^{(1)}(\alpha\beta\gamma) J_\sigma \ , \quad J_\sigma = \sum_\rho D_{\sigma\rho}^{(1)*}(\alpha\beta\gamma) \overline{J}_\rho \ , \tag{6-76}$$

where $D^{(1)}$ is the irreducible matrix for $j = 1$ (for an explicit expression see Rose 1957). From (5-264) we obtain the relation between the matrix elements of J_ρ and $\overline{J}_\rho$

$$\langle jm'|J_\rho|jm\rangle = \langle jm|\overline{J}_\rho|jm'\rangle \ . \tag{6-77}$$

According to angular momentum theory (Rose 1957) and (6-77),

$$\langle jm|J_z|jm\rangle = \langle jm|\overline{J}_z|jm\rangle = m \ , \tag{6-78a}$$

$$\langle jm \pm 1|J_x \pm iJ_y|jm\rangle = \langle jm|\overline{J}_x \pm i\overline{J}_y|jm \pm 1\rangle = [(j \mp m)(j \pm m + 1)]^{1/2} \ . \tag{6-78b}$$

We stress that (6-78a) does not imply $\overline{J}_z = J_z$ and (6-78b) does not mean $(\overline{J}_x \pm i\overline{J}_y) = (J_x \pm iJ_y)^\dagger$. This point will become more clear by rewriting (6-78) in the following form:

$$\langle \psi_m^{(j)}|J_z|\psi_m^{(j)}\rangle = \langle \psi^{(j)m}|\overline{J}_z|\psi^{(j)m}\rangle \ , \tag{6-79a}$$

$$\langle \psi_{m\pm1}^{(j)}|J_x \pm iJ_y|\psi_m^{(j)}\rangle = \langle \psi^{(j)m}|\overline{J}_x \pm i\overline{J}_y|\psi^{(j)m\pm1}\rangle \ , \tag{6-79b}$$

where $\psi_m^{(j)}$ and $\psi^{(j)m}$ are the $SO_3 \supset SO_2$ and $\overline{SO}_3 \supset \overline{SO}_2$ irreducible basis, respectively.

6.8.2. Irreducible tensors $T_m^{(\nu)}$ of SO_3 and $\overline{SO}_3$ in general cases

SO_3 is a simply reducible group, therefore the multiplicity label θ in (5-261) is redundant. The reduced matrix element of the angular momentum J is (see Rose 1957)

$$\langle j\|J\|j\rangle = \sqrt{j(j+1)} \ . \tag{6-80}$$

From (5-250), (5-253), (5-261) and (6-80) we obtain the definition for the irreducible tensors of SO_3 and $\overline{SO}_3$,

$$[J_\rho, T_m^{(\nu)}] = \sum_t D_{tm}^{(\nu)}(J_\rho)T_t^{(\nu)} = \sqrt{\nu(\nu+1)}C_{\nu m,1\rho}^{\nu,m+\rho}T_{m+\rho}^{(\nu)} \ , \tag{6-81a}$$

$$[\overline{J}_\rho, \overline{T}_m^{(\nu)}] = -\sum_t D_{tm}^{(\nu)}(J_\rho)\overline{T}_t^{(\nu)} = -\sqrt{\nu(\nu+1)}C_{\nu m,1\rho}^{\nu,m+\rho}\overline{T}_{m+\rho}^{(\nu)} \ , \tag{6-81b}$$

where $\nu = j$. From (6-81) one has

$$[J_\rho, J_\sigma] = -\sqrt{2}C_{1\rho,1\sigma}^{1,\rho+\sigma}J_{\rho+\sigma} \ , \tag{6-82a}$$

$$[\overline{J}_\rho, \overline{J}_\sigma] = \sqrt{2}C_{1\rho,1\sigma}^{1,\rho+\sigma}\overline{J}_{\rho+\sigma} \ . \tag{6-82b}$$

Using the expression for the CG coefficients of SO_3 (see Rose 1957), one obtains from (6-81)

$$\begin{aligned}
&[J_z, T_m^{(\nu)}] = mT_m^{(\nu)} \ , \quad [\overline{J}_z, \overline{T}_m^{(\nu)}] = -m\overline{T}_m^{(\nu)} \ , \\
&[J_x \pm iJ_y, T_m^{(\nu)}] = [(\nu \mp m)(\nu \pm m + 1)]^{1/2}T_{m\pm1}^{(\nu)} \ , \\
&[\overline{J}_x \pm i\overline{J}_y, \overline{T}_m^{(\nu)}] = -[(\nu \mp m)(\nu \pm m + 1)]^{1/2}\overline{T}_{m\pm1}^{(\nu)} \ .
\end{aligned} \tag{6-83}$$

From (5-262) and (5-263) it follows that

$$[J_\rho, D^{(j)}_{mk}(\alpha\beta\gamma)] = -\sqrt{j(j+1)}C^{jm}_{jm-\rho,1\rho}D^{(j)}_{m-\rho,k}(\alpha\beta\gamma) \ , \tag{6-84a}$$

$$[\overline{J}_\rho, D^{(j)}_{mk}(\alpha\beta\gamma)] = -\sqrt{j(j+1)}C^{jk+\rho}_{jk,1\rho}D^{(j)}_{m,k+\rho}(\alpha\beta\gamma) \ , \tag{6-84b}$$

$$[J_\rho, D^{(j)*}_{mk}(\alpha\beta\gamma)] = \sqrt{j(j+1)}C^{jm+\rho}_{jm,1\rho}D^{(j)*}_{m+\rho,k}(\alpha\beta\gamma) \ , \tag{6-85a}$$

$$[\overline{J}_\rho, D^{(j)*}_{mk}(\alpha\beta\gamma) = \sqrt{j(j+1)}C^{jk}_{jk-\rho,1\rho}D^{(j)*}_{m,k-\rho}(\alpha\beta\gamma) \ . \tag{6-85b}$$

One sees, by comparing (6-81) with (6-84) and (6-85), that

$$D^{(j)*}_{mk}(\alpha\beta\gamma) = T^{(j)}_m \ , \quad D^{(j)}_{mk}(\alpha\beta\gamma) = \overline{T}^{(j)}_k \ . \tag{6-86a,b}$$

From (6-86a) it is seen that there are $2j+1$ independent tensor operators $T^{(j)}$ with the same irrep label j, which are enumerated by assigning a distinct intrinsic quantum number k to each of them. This is consistent with a theorem proved by Louck (1970) which asserts that the number of the linearly independent irreducible tensor operators belonging to the same irrep (ν) equals the dimension of the irrep.

Now let us look at the physical meaning of the intrinsic irreducible tensor defined by (6-81b). Using (6-87), (6-84b) and (6-81), it can be shown that if the irreducible tensor $T^{(\nu)}_m$ of SO_3 is a scalar under rotation $\overline{R}(\alpha\beta\gamma)$ about the intrinsic axes,

$$[\overline{J}_\rho, T^{(\nu)}_m] = 0 \ , \tag{6-87}$$

then the tensor

$$T'^{(\nu)}_m = \sum_{m'} D^{(\nu)}_{m'm}(\alpha\beta\gamma)T^{(\nu)}_{m'} \tag{6-88}$$

is the intrinsic irreducible tensor $\overline{T}^{(\nu)}_m$. $T'^{(\nu)}_m$ is nothing else but the operator $T^{(\nu)}_m$ expressed in the intrinsic frame.

Some important operators in physics satisfy the requirement (6-87); these include the angular momentum operator $T^{(1)}_\rho = J_\rho$ and the multipole operator

$$T^{(\lambda)}_\mu = \sum_{i=1}^{A} r_i^\lambda Y_{\lambda\mu}(\theta_i\varphi_i) \ . \tag{6-89}$$

The corresponding intrinsic irreducible tensors are

$$J'_\rho = \overline{J}_\rho \ ,$$

$$T'^{(\lambda)}_\mu = \overline{T}^{(\lambda)}_\mu = \sum_{i=1}^{A} r'^\lambda_i Y_{\lambda\mu}(\theta'_i\varphi'_i) \ , \tag{6-90}$$

where $r_i, \theta_i, \varphi_i (r'_i, \theta'_i, \varphi'_i)$ are the coordinates of the i–th particle in the fixed (intrinsic) frame.

Note that $T'^{(\nu)}_m$ as defined by (6-88) is in general not necessarily an intrinsic irreducible tensor $\overline{T}^{(\nu)}_m$, since the transformation property $[\overline{J}_\rho, T'^{(\nu)}_m]$ of $T'^{(\nu)}_m$ under the intrinsic rotation also depends on the transformation property $[\overline{J}_\rho, T^{(\nu)}_m]$ of the tensor $T^{(\nu)}_m$ under the intrinsic rotation and there is no direct connection between $[\overline{J}_\rho, T'^{(\nu)}_m]$ and $[\overline{J}_\rho, T^{(\nu)}_m]$. For example, suppose that $T^{(\nu)}_m = D^{(\nu)*}_{mk_0}(\alpha\beta\gamma)$, with k_0 fixed. From (6-88) it is seen that

$$T'^{(\nu)}_m = \delta_{m,k_0} \ .$$

Therefore $T'^{(\nu)}_m$ is a scalar with respect to either the external or intrinsic rotation, rather than the intrinsic irreducible tensor $\overline{T}^{(\nu)}_m$.

We have made abstract the concept of the intrinsic group from the concrete physical problem, and then turned back to use it in treating the problem of the collective rotation of nuclei about the intrinsic axes. Some puzzling aspects of the problem now become transparent. All the relations given by Bohr (1975, Appendix IA–b) have been easily obtained in this chapter as special cases of the results in the previous chapter. So it may be said that the intrinsic group $\overline{SO}_3$ provides an appropriate mathematical formalism for the description of nuclear rotation about the intrinsic axes.

Chapter 7

The Unitary Groups

Unitary groups are extensively applied in physics. The applications fall mainly into the following two categories.

1. The unitary group is the symmetry group or approximate symmetry group of the Hamiltonian of a system. In such a case, an eigenfunction of the Hamiltonian belongs to a certain irrep of the unitary group and thus the states of the system can be labelled by the irrep labels of the unitary group and its subgroups. For example, the Hamiltonian of a nucleus has SU_2 symmetry due to the charge independence of the nuclear force if the Coulomb forces between protons are neglected, so the nuclear energy levels are characterized by the isospin T and its third component T_z, which are the irrep labels of SU_2 and SO_2, respectively. The Hamiltonian of a nucleus exhibits SU_4 symmetry if the two-body interaction does not depend on the spin and isospin of the two nucleons, as is for light nuclei. An isotropic harmonic oscillator in three-dimensional space has SU_3 symmetry. Elementary particles obey approximate SU_3, SU_4, or SU_5 symmetry in flavor space, and SU_3 symmetry in color space.

2. The unitary group is not a symmetry group of the Hamiltonian. In such cases the purpose of introducing the unitary group is to define a complete set of basis functions classified according to the irreps of the unitary group and its subgroups, so that the Hamiltonian can be conveniently diagonalized in this basis. If the symmetry group G of the Hamiltonian is a subgroup of SU_n, we will naturally choose the $SU_n \supset G$ irreducible basis to facilitate the diagonalization. For example we use the group chains $SU_{2l+1} \supset SO_{2l+1} \supset SO_3$ or $SU_{2j+1} \supset Sp_{2j+1} \supset SO_3$ and $SU_4 \supset SU_2 \times SU_2$ in the nuclear shell model.

The rep theory for the unitary group to be introduced below can be easily extended to the so-called *graded* (or *super*) *unitary group* $SU(m/n)$ (Chen & Chen 1983, Chen, Gao and Chen 1984).

7.1. Unitary Groups in Coordinate Space and State Space

Suppose that there are f particles with the coordinate indices $a_j = 1, 2, \ldots, f$ and n single particle states $m_1, m_2, \ldots, m_n$ (or $\alpha, \beta, \gamma, \ldots \delta$). We use $i_j (j = 1, 2, \ldots, f)$ to denote any one of the states $m_1, \ldots, m_n$. The n single particle states $\varphi_{m_1}, \varphi_{m_2}, \ldots, \varphi_{m_n}$ span the space V_n, the fundamental rep space of the unitary group $\mathcal{U}_n$ or $S\mathcal{U}_n$ in state space. Under the operation of the group element $\mathcal{R}(b)$ of $\mathcal{U}_n$ they transform as

$$\mathcal{R}(b)\varphi_{m_i} = \sum_{j=1}^{n} \mathcal{D}_{ji}(b)\varphi_{m_j} , \quad \mathcal{D}_{ji} \equiv R_{ij} , \tag{7-1}$$

where b are the group parameters, and $\mathcal{D}(b)$ is an $n \times n$ unitary matrix. The operator $\mathcal{R}(b)$ is given in (5-95) with parameter a replaced by b. The state φ_m is a tensor of rank one.

The n^f f–particle product states are designated by

$$|i_1 i_2 \dots i_f\rangle = \varphi_{i_1}^{a_1} \varphi_{i_2}^{a_2} \dots \varphi_{i_f}^{a_f} \ , \quad i_1, i_2, \dots, i_f = m_1, m_2, \dots m_n \ . \tag{7-2}$$

The action of the group element $\mathcal{R}(b)$ on the f–particle product states is defined in (5-96a)

$$\mathcal{R}(b)|i_1 i_2 \dots i_f\rangle = \sum_{i_1' i_2' \dots i_f'} \mathcal{D}_{i_1' i_1}(b) \dots \mathcal{D}_{i_f' i_f}(b) |i_1' i_2' \dots i_f'\rangle \ . \tag{7-3}$$

It follows that the n^f product states (7-2) form an f–th rank tensor in n–dimensional space. The space spanned by (7-2) is called the *tensor space*, hereafter denoted by V_n^f, and it generates a reducible rep for both the group $\mathcal{U}_n$ and for the group S_f.

The elements $\mathcal{R}(b)$ of the unitary group acting on many–particle states are given in (5-96).

Letting the group parameter $b_{\alpha\beta} = \varepsilon$ be infinitesimal, and setting all other parameters $b_{\alpha'\beta'} = 0$ for $\alpha' \neq \alpha$ and $\beta' \neq \beta$, from (5-96c) and (5-94b) we obtain

$$\begin{aligned} \mathcal{E}_{\alpha\beta}(\varphi_{i_1}^{a_1} \varphi_{i_2}^{a_2} \dots \varphi_{i_f}^{a_f}) = \delta_{i_1\beta} \varphi_\alpha^{a_1} \varphi_{i_2}^{a_2} \dots \varphi_{i_f}^{a_f} + \delta_{i_2\beta} \varphi_{i_1}^{a_1} \varphi_\alpha^{a_2} \dots \varphi_{i_f}^{a_f} + \dots \\ + \delta_{i_f\beta} \varphi_{i_1}^{a_1} \varphi_{i_2}^{a_2} \dots \varphi_\alpha^{a_f} \ . \end{aligned} \tag{7-4}$$

We may note that (7-10) still holds when some a_i's are equal. $\mathcal{E}_{\alpha\alpha}$ is the number operator for the state α,

$$\hat{n}_\alpha = \mathcal{E}_{\alpha\alpha} = \sum_{i=1}^{f} c_\alpha^\dagger(a_i) c_\alpha(a_i) \ . \tag{7-5}$$

Analogously, we can define the unitary group U_n or SU_n in coordinate space. The single particle states $\varphi_m^{a_i} (i = 1, 2, \dots, n)$ carry the fundamental rep of U_n. Under the action of the group element $R(b)$ of U_n, $\varphi_m^{a_i}$ transform as

$$R(b) \varphi_m^{a_i} = \sum_{j=1}^{n} \mathcal{D}_{ji}(b) \varphi_m^{a_j} \ . \tag{7-6}$$

The infinitesimal operators of U_n are

$$E_{a_1 a_2} = \sum_{\alpha=1}^{n} e_{a_1 a_2}^{(\alpha)} \ , \tag{7-7}$$

$$e_{a_1 a_2}^{(\alpha)} = c_\alpha^\dagger(a_1) c_\alpha(a_2) \ . \tag{7-8}$$

The operator $e_{a_1 a_2}^{(\alpha)}$ changes the coordinate index a_2 into a_1 of a particle in the state α,

$$e_{a_1 a_2}^{(\alpha)} \varphi_\beta^{a_3} = \delta_{\alpha\beta} \delta_{a_2 a_3} \varphi_\alpha^{a_1} \ . \tag{7-9}$$

In parallel to (5-94d), (5-97) and (7-4), we have

$$[e_{ab}^{(\alpha)}, e_{cd}^{(\beta)}] = \delta_{\alpha\beta} (\delta_{bc} e_{ad}^{(\alpha)} - \delta_{ad} e_{cb}^{(\alpha)}) \ , \tag{7-10}$$

$$[E_{ab}, E_{cd}] = \delta_{bc} E_{ad} - \delta_{ad} E_{cb} \ . \tag{7-11}$$

$$\begin{aligned} & E_{ab}(\varphi_{i_1}^{a_1} \varphi_{i_2}^{a_2} \dots \varphi_{i_n}^{a_n}) \\ & = \delta_{a_1 b} \varphi_{i_1}^{a} \varphi_{i_2}^{a_2} \dots \varphi_{i_n}^{a_n} + \delta_{a_2 b} \varphi_{i_1}^{a_1} \varphi_{i_2}^{a} \dots \varphi_{i_n}^{a_n} + \dots + \delta_{a_n b} \varphi_{i_1}^{a_1} \varphi_{i_1}^{a_2} \dots \varphi_{i_n}^{a} \ . \end{aligned} \tag{7-12}$$

As in Chapter 4, we may define the coordinate permutation group S_f and the state permutation group $\mathcal{S}_f$, which permute the subscripts of a and those of i, respectively. Obviously, the groups defined in different spaces commute, that is,

$$[S_f, \mathcal{S}_f] = 0 \,, \quad [U_n, \mathcal{U}_n] = 0 \,, \tag{7-13}$$

$$[S_f, \mathcal{U}_n] = 0 \,, \quad [\mathcal{S}_f, U_n] = 0 \,, \tag{7-14}$$

and the groups defined in the same space do not commute,

$$[S_f, U_n] \neq 0 \,, \quad [\mathcal{S}_f, \mathcal{U}_n] \neq 0 \,. \tag{7-15}$$

We know that the state permutation operators $\wp$ of $\mathcal{S}_f$ have definite meaning when acting on the product state (7-2) with all the single particle state $i_1, i_2, \ldots, i_f$ different. However, after the action of the group elements of $\mathcal{U}_n$ on the product states, identical single particle states will occur in the product states and the permutation operator $\wp$ becomes meaningless (only the class operators of $\mathcal{S}_f$ remain meaningful). Therefore $\mathcal{S}_f$ does not commute with $\mathcal{U}_n$.

7.2. Relations Between Unitary and Permutation Groups

7.2.1. The Gel'fand invariants

The following n operators were introduced by Gel'fand (1950)

$$\mathfrak{I}_k^{(n)} = \sum_{i_1 i_2, \ldots i_k = 1}^{n} \mathcal{E}_{i_1 i_2} \mathcal{E}_{i_2 i_3} \ldots \mathcal{E}_{i_k i_1} \,, \quad k = n, n-1, \ldots, 1 \,. \tag{7-16}$$

It can be proved that the $\mathfrak{I}_k^{(n)}$ satisfy condition (5-219), that is,

$$[\mathcal{E}_{ij}, \mathfrak{I}_k^{(n)}] = 0 \,, \quad i, j = 1, 2, \ldots, n \,. \tag{7-17}$$

Consequently, $\{\mathfrak{I}_k^{(n)}\}$ is a set of invariants of $\mathcal{U}_n$. $\mathfrak{I}_1^{(n)}$ is the number operator

$$\mathfrak{I}_1^{(n)} = \sum_{i=1}^{n} \mathcal{E}_{ii} = f \,. \tag{7-18}$$

Gel'fand showed that the eigenvalues of the n invariants $\{\mathfrak{I}_k^{(n)}\}$ uniquely label an irrep of $\mathcal{U}_n$; therefore, $\{\mathfrak{I}_k^{(n)}\}$ is the CSCO-I of $\mathcal{U}_n$.

From (5-124), the infinitesimal operators of $S\mathcal{U}_n$ are known to be

$$\mathcal{E}'_{ij} = \mathcal{E}_{ij} - \delta_{ij} \frac{1}{n} \sum_{k=1}^{n} \mathcal{E}_{kk} \,. \tag{7-19}$$

The CSCO-I of $S\mathcal{U}_n$ consists of the $n-1$ invariants

$$\mathfrak{I}'^{(n)}_k = \sum_{i_1 i_2 \ldots i_k = 1}^{n} \mathcal{E}'_{i_1 i_2} \mathcal{E}'_{i_2 i_3} \ldots \mathcal{E}'_{i_k i_1} \,, \quad k = n, n-1, \ldots, 2 \,. \tag{7-20}$$

$\mathfrak{I}'^{(n)}_k$ can be expressed in terms of $\mathfrak{I}_k^{(n)}$. For example, from (7-19) we have [Cf. (5-222b)]

$$\mathfrak{I}'^{(n)}_1 = 0 \,, \quad \mathfrak{I}'^{(n)}_2 = \mathfrak{I}_2^{(n)} - \frac{1}{n} \left(\sum_{i=1}^{n} \mathcal{E}_{ii} \right)^2 = \mathfrak{I}_2^{(n)} - \frac{f^2}{n} \,. \tag{7-21}$$

The above relations also hold for the unitary group U_n or SU_n in coordinate space.

In view of the functional relationship between the CSCO–I of $S\mathcal{U}_n$ and $\mathcal{U}_n$, any eigenfunction $\psi^{(\nu)}$ of the CSCO–I of $\mathcal{U}_n$ is necessarily an eigenfunction of the CSCO–I of $S\mathcal{U}_n$, and thus if $\psi^{(\nu)}$ belongs to the irrep (ν) of $\mathcal{U}_n$, it also belongs to an irrep of $S\mathcal{U}_n$, and vice versa. In the following we will prove that irreps of $\mathcal{U}_n$ remain irreducible when we go to the subgroup $S\mathcal{U}_n$.

From (7-3) it is known that the irreducible matrix elements $D^{(\nu)}(\mathcal{R})$ of an irrep (ν) of $\mathcal{U}_n$ are homogeneous polynomials of degree f in the transformation matrix elements R_{ij},

$$D^{(\nu)}(\mathcal{R}) = F^{(\nu)}(R_{ij}) \ . \tag{7-22}$$

The unitary transformation (R_{ij}) can be made unimodular by the scale transformation

$$R_{ij} = (\det R)^{1/n} R'_{ij} \ . \tag{7-23}$$

From (7-22) and (7-23) we know that the representation matrices of $\mathcal{U}_n$ and those of $S\mathcal{U}_n$ are related by the following

$$D^{(\nu)}(\mathcal{U}_n) = (\det R)^{f/n} D^{(\nu)}(S\mathcal{U}_n) \ . \tag{7-24}$$

Therefore an irrep (ν) of $\mathcal{U}_n$ remains irreducible for $S\mathcal{U}_n$.

7.2.2. The relation between CSCO–I's of unitary and permutation groups

Partensky (1972) defined the operators

$$P_k^{a_1 a_2 \ldots a_k} = \frac{1}{k!} \sum_{i_1 i_2 \ldots i_k = 1}^{n} (e_{i_1 i_2}^{(a_1)} e_{i_2 i_3}^{(a_2)} \ldots e_{i_k i_1}^{(a_k)})_s \ , \tag{7-25}$$

where the subscript s means symmetrization in the indices $a_1, a_2, \ldots a_k$,

$$(e_{i_1 i_2}^{(a_1)} e_{i_2 i_3}^{(a_2)} \ldots e_{i_k i_1}^{(a_k)})_s = \sum_{p \in S_k} p(e_{i_1 i_2}^{(a_1)} e_{i_2 i_3}^{(a_2)} \ldots e_{i_k i_1}^{(a_k)}) \ . \tag{7-26}$$

We now prove that acting on the basis $\varphi_{m_1}^{a_1} \varphi_{m_2}^{a_2} \ldots \varphi_{m_k}^{a_k}$, $P_k^{a_1 a_2 \ldots a_k}$ is equivalent to the average k-cycle class operator $C^{(k)}(k)$ of S_k,

$$P_k^{a_1 a_2 \ldots a_k} = C^{(k)}(k) = \frac{1}{(k-1)!} C_{(k)}(k) \ . \tag{7-27}$$

From (5-94b) we have

$$\sum_{i_1 i_2 = 1}^{n} e_{i_1 i_2}^{(a_1)} e_{i_2 i_1}^{(a_2)} \varphi_{m_1}^{(a_1)} \varphi_{m_2}^{(a_2)} = \sum_{i_1 i_2 = 1}^{n} \delta_{i_1 m_2} \delta_{i_2 m_1} \varphi_{i_1}^{(a_1)} \varphi_{i_2}^{(a_2)} = \varphi_{m_2}^{(a_1)} \varphi_{m_1}^{(a_2)} \ . \tag{7-28}$$

Therefore

$$\sum_{i_1 i_2 = 1}^{n} e_{i_1 i_2}^{(a_1)} e_{i_2 i_1}^{(a_2)} = (a_1 a_2) \ . \tag{7-29a}$$

It is easy to show that in general we have

$$\sum_{i_1 i_2 \ldots i_k = 1}^{n} e_{i_1 i_2}^{(a_1)} e_{i_2 i_3}^{(a_2)} \ldots e_{i_k i_1}^{(a_k)} = (a_1 a_2 \ldots a_k) \ . \tag{7-29b}$$

A symmetrization of (7-29b) gives rise to (7-27). For example,

$$P_3^{a_1 a_2 a_3} = \tfrac{1}{2} C_{(3)}(3) = \tfrac{1}{2} \left[(123) + (132) \right] \ .$$

Partensky (1972) defined another operator

$$P_k^f = \binom{f}{k}^{-1} \sum_{a_1>\ldots>a_k=1}^{f} P_k^{a_1 a_2 \ldots a_k} = \frac{1}{g_{(k)}} C_{(k)}(f) ,$$
$$g_{(k)} = \binom{f}{k}(k-1)! , \tag{7-30}$$

where $C_{(k)}(f)$ is the k-cycle class operator of S_f, and $g_{(k)}$ is the number of elements in the class. For example

$$P_3^4 = \frac{1}{4}[P_3^{a_1 a_2 a_3} + P_3^{a_1 a_2 a_4} + P_3^{a_1 a_3 a_4} + P_3^{a_2 a_3 a_4}]$$
$$= \frac{1}{8}[(123) + (132) + (124) + (142) + (134) + (143) + (234) + (243)] .$$

Now we turn to derive a relation between P_k^f and the invariants of $\mathcal{U}_n$. From (7-30), (7-25) and (7-16) we have

$$P_2^f = \binom{f}{2}^{-1} \sum_{i_1 i_2=1}^{n} \sum_{a_1>a_2=1}^{f} e_{i_1 i_2}^{(a_1)} e_{i_2 i_1}^{(a_2)} = \frac{1}{f(f-1)} \sum_{i_1 i_2=1}^{n} \left[\sum_{a_1 a_2=1}^{f} e_{i_1 i_2}^{(a_1)} e_{i_2 i_1}^{(a_2)} - \sum_{a_1=1}^{f} e_{i_1 i_2}^{(a_1)} e_{i_2 i_1}^{(a_1)} \right]$$
$$= \frac{1}{f(f-1)} \left[\Im_2^{(n)} - n \sum_{i_1=1}^{n} \sum_{a_1=1}^{f} e_{i_1 i_1}^{(a_1)} \right] = \frac{1}{f(f-1)} [\Im_2^{(n)} - nf] . \tag{7-31}$$

Let us introduce the function

$$F^{(n)} = \prod_{j>i=1}^{n} (1 - \delta_{a_i a_j}) . \tag{7-32a}$$

For example

$$F^{(3)} = 1 - (\delta_{a_1 a_2} + \delta_{a_1 a_3} + \delta_{a_2 a_3}) + 2\delta_{a_1 a_2}\delta_{a_2 a_3} . \tag{7-32b}$$

Combining (7-30), (7-25), (7-32), (5-94c) and (7-16),

$$P_3^f = \frac{1}{f(f-1)(f-2)} \sum_{i_1 i_2 i_3=1}^{n} \sum_{a_1>a_2>a_3=1}^{f} (e_{i_1 i_2}^{a_1} e_{i_2 i_3}^{a_2} e_{i_3 i_1}^{a_3})_s$$
$$= \frac{1}{f(f-1)(f-2)} \sum_{i_1 i_2 i_3=1}^{n} \sum_{a_1 a_2 a_3=1}^{f} e_{i_1 i_2}^{a_1} e_{i_2 i_3}^{a_2} e_{i_3 i_1}^{a_3} F^{(3)}$$
$$= [\Im_3^{(n)} - 2n\Im_2^{(n)} + (n^2+1)f - f^2]/[f(f-1)(f-2)] , \tag{7-33}$$

where we used $\sum_{i_1=1}^{n} \sum_{a_1=1}^{f} e_{i_1 i_1}^{(a_1)} = \sum_{i=1}^{n} n_i = f, n_i$ being the number of particles in the state i [see (7-11)].

According to (7-30), (7-31) and (7-33) we obtain

$$\Im_2^{(n)} = 2C_{(2)}(f) + nf ,$$
$$\Im_3^{(n)} = 3C_{(3)}(f) + 4nC_{(2)}(f) + (n^2-1)f + f^2 . \tag{7-34}$$

In the same way we can prove that in the tensor space V_n^f, $\Im_k^{(n)}$ is a function of the class operators $C_{(k)}(f), \ldots, C_{(2)}(f)$ of S_f, that is,

$$\Im_k^{(n)} = F_k^{(n)}(C_{(k)}(f) , C_{(k-1)}(f), \ldots, C_{(2)}(f)) . \tag{7-35}$$

It was noted in Sec. 3.2 that all the class operators of S_f are functions of the CSCO–I of S_f. Furthermore, the CSCO–I of S_f and $\mathcal{S}_f$ are equal, $C(f)$[1] $= \mathcal{C}(f)$, therefore the invariants of $\mathcal{U}_n$ are functions of $C(f)$ or $\mathcal{C}(f)$,

$$\Im_k^{(n)} = F_k^{(n)}(C(f)) = F_k^{(n)}(\mathcal{C}(f)) \ . \tag{7-36}$$

Analogously, it can be shown that the invariants $I_k^{(n)}$ of U_n are functions of the CSCO–I of S_f, that is, $I_k^{(n)} = F_k^{(n)}(C(f))$. Combining it with (7-36) leads to an important relation

$$I_k^{(n)} = \Im_k^{(n)} = F_k^{(n)}(C(f)) = F_k^{(n)}(\mathcal{C}(f)) \ . \tag{7-37}$$

In other words, in a tensor space, among the CSCO's $\{I_k^{(n)}\}, \{\Im_k^{(n)}\}, C(f)$ and $\mathcal{C}(f)$ of the four groups $U_n, \mathcal{U}_n, S_f$ and $\mathcal{S}_f$, only one is functionally independent. Therefore in the space V_n^f, an eigenfunction of any one of the four CSCO's must be an eigenfunction of the other three CSCO's. Thus we can use the same irrep label (ν) for the four groups $U_n, \mathcal{U}_n, S_f$ and $\mathcal{S}_f$ and we have the following theorem:

Theorem 7.1: In the tensor space V_n^f, if $\psi^{(\nu)}$ belongs to the irrep (ν) of one of the four groups $U_n, \mathcal{U}_n, S_f$ and $\mathcal{S}_f$, then $\psi^{(\nu)}$ also belongs to the irrep (ν) of any one of the other three groups.

There are a variety of ways to label the irreps of the four groups. The most extensively used is the partition

$$[\nu] = [\nu_1 \nu_2 \ldots \nu_n] = [m_{in}] \equiv [m_{1n}, m_{2n}, \ldots, m_{nn}] \ .$$

We may use the eigenvalues of $C(f)$ or $I_k^{(n)}$ as the irrep label as well. Partensky (1972) proved that the eigenvalues of $I_k^{(n)}$ are related to the partition through the following

$$I_k^{(n)} = \sum_{i=1}^{n} m_{in} f_k^{(n)}(i) \ , \tag{7-38a}$$

where $f_k^{(n)}(i)$ is obtained from the recursive formula

$$\begin{aligned} f_{k+1}^{(n)}(i) &= q_{in} f_k^{(n)}(i) - \sum_{j=1}^{i-1} f_k^{(n)}(j) \ , \\ q_{in} &= m_{in} + n - i \ , \quad f_1^{(n)}(i) \equiv 1 \ . \end{aligned} \tag{7-38b}$$

For example

$$I_1^{(n)} = f \ , \quad I_2^{(n)} = \sum_{i=1}^{n} m_{in}(m_{in} - 2i + n + 1) \ . \tag{7-38c}$$

From (7-38c), (7-34) and (7-37) we obtain the eigenvalues of the two– and three–cycle class operators as functions of the partition

$$\begin{aligned} \lambda_{(2)}(f) &= \frac{f}{2} + \frac{1}{2} \sum_i \nu_i(\nu_i - 2i) \ , \\ \lambda_3(f) &= \tfrac{1}{3} \Big\{ 2f - \tfrac{3}{2} f^2 + \sum_i \nu_i \left[\nu_i^2 - \left(3i - \tfrac{3}{2}\right) \nu_i + 3i(i-1) \right] \Big\} \ . \end{aligned} \tag{7-38d}$$

[1] In Secs. 7.2–7.5, $C(f)$ represents the CSCO–I of S_f, while $C_{(k)}(f)$ represents the k–cycle class operators of S_f.

7.2.3 Relations between the generators of unitary and permutation groups

Suppose the coordinates of the particles are all different. From (7-29a) we obtain the coordinate permutation operator

$$p_{ab} = \sum_{\alpha,\beta=1}^{n} e^{(a)}_{\alpha\beta} e^{(b)}_{\beta\alpha} \,. \tag{7-39a}$$

Setting $n = 2$ in (7-39a) and using the Pauli matrices [Eq. (5-122)]

$$\begin{aligned} &\sigma_x = e_{12} + e_{21} \,, \quad \sigma_y = i(e_{21} - e_{12}) \,, \\ &\sigma_z = (e_{11} - e_{22}) \,, \quad 1 = e_{11} + e_{22} \,, \end{aligned} \tag{7-39b}$$

we obtain the well known Dirac equality

$$p_{ab} = \frac{1}{2}(1 + \boldsymbol{\sigma}_a \cdot \boldsymbol{\sigma}_b) \,. \tag{7-39c}$$

Expressed in terms of the generators of $S\mathcal{U}_n$, (7-39a) reads

$$\begin{aligned} p_{ab} &= \sum_{\alpha,\beta=1}^{n} e'^{(a)}_{\alpha\beta} e'^{(b)}_{\beta\alpha} + \frac{1}{n} \,, \\ e'_{\alpha\beta} &= e_{\alpha\beta} - \delta_{\alpha\beta} \frac{1}{n} \sum_{\gamma} e_{\gamma\gamma} \,. \end{aligned} \tag{7-39d}$$

Equation (7-39d) is the extension of Dirac's equality (7-39c).

The relation between the generators p_{ab} of S_f and E_{ab} of U_n is

$$E_{ab} E_{ba} = 1 + p_{ab} \,. \tag{7-40}$$

This may be verified directly by applying it to the state $\varphi^a_\alpha \varphi^b_\beta$ and noting (7-12).

When the single particle states are all different, the state permutation operator $\wp_{\alpha\beta}$ is expressed as

$$\wp_{\alpha\beta} = \sum_{a,b=1}^{f} e^{(\alpha)}_{ab} e^{(\beta)}_{ba} \,, \tag{7-41}$$

and the counterpart of (7-40) is

$$\mathcal{E}_{\alpha\beta} \mathcal{E}_{\beta\alpha} = 1 + \wp_{\alpha\beta} \,. \tag{7-42}$$

From (7-40) and (7-42), one also sees that S_f does not commute with U_n, and $\mathcal{S}_f$ does not commute with $\mathcal{U}_n$.

7.3. The CSCO–II and CSCO–III of U_n and SU_n

The following discussion is equally valid for the unitary groups in coordinate space and state space. We assume here, for convenience, that U_n stands for the unitary group in state space.

The group U_n has $r = n^2$ parameters, therefore we need to find n^2 commuting operators to form the CSCO–III of U_n. We are going to show that the CSCO of the group chain

$$U_n \supset U_{n-1} \supset \ldots \supset U_2 \supset U_1 \tag{7-43}$$

and the CSCO of the corresponding intrinsic group chain

$$\overline{U}_n \supset \overline{U}_{n-1} \supset \ldots \supset \overline{U}_2 \supset \overline{U}_1 \tag{7-44}$$

constitute the CSCO–III of U_n.

According to (5-236), U_n and its intrinsic group $\overline{U}_n$ have the same CSCO, which provides n commuting operators

$$I_k^{(n)} = \overline{I}_k^{(n)} , \quad k = n, n-1, \ldots, 2, 1 . \tag{7-45a}$$

$$I_k^{(n)} = \sum_{i_1 \ldots i_k = 1}^{n} E_{i_1 i_2} E_{i_2 i_3} \ldots E_{i_k i_1} . \tag{7-45b}$$

We still use C to represent the CSCO–I,

$$C = \{I_k^{(n)}\} \equiv \left(I_n^{(n)}, I_{n-1}^{(n)}, \ldots, I_2^{(n)}, I_1^{(n)}\right) , \tag{7-46}$$

and use $C(s)$ and $\overline{C}(s)$ to represent the CSCO of the subgroup chains (7-43) and (7-44),

$$\begin{aligned} C(s) &= \left(\{I_k^{(n-1)}\}, \ldots, \{I_k^{(2)}\}, I_1^{(1)}\right) , \\ \overline{C}(s) &= \left(\{\overline{I}_k^{(n-1)}\}, \ldots, \{\overline{I}_k^{(2)}\}\, \overline{I}_1^{(1)}\right) , \end{aligned} \tag{7-47a}$$

where

$$\begin{aligned} I_k^{(m)} &= \sum_{i_1 \ldots i_k = 1}^{m} E_{i_1 i_2} E_{i_2 i_3} \ldots E_{i_k i_1} , \\ \overline{I}_k^{(m)} &= \sum_{i_1 \ldots i_k = 1}^{m} \overline{E}_{i_1 i_2} \overline{E}_{i_2 i_3} \ldots \overline{E}_{i_k i_1} . \end{aligned} \qquad m = n-1, \ldots, 2, 1 . \tag{7-47b}$$

$C(s)$ contains $\sum_{m=1}^{n-1} m = \frac{1}{2} n(n-1)$ operators. Therefore the set of operators

$$K = \left(C, C(s), \overline{C}(s)\right) \tag{7-48}$$

contains n^2 operators. It is easy to show that the n^2 operators commute with one another. Gel'fand proved that they are independent. Therefore K is the CSCO–III of U_n, and the group chain (7-43) is a canonical group chain.

Similarly, it can be shown that a canonical group chain of SU_n is

$$SU_n \supset SU_{n-1} \times U_1 \supset SU_{n-2} \times U_1 \supset \ldots \supset SU_2 \times U_1 \supset U_1 . \tag{7-49}$$

SU_n and $\overline{SU}_n$ have the same CSCO which contains $n-1$ operators:

$$C = \{I'^{(n)}_k\} = \left(I'^{(n)}_n, I'^{(n)}_{n-1}, \ldots, I'^{(n)}_2\right) . \tag{7-50}$$

Each link $SU_l \times U_1$ in the group chain (7-49) provides l operators, those are the $l-1$ operators of the CSCO of SU_l and the CSCO $E_{l+1,l+1}$ of the group U_1 which acts on the single particle state φ_{l+1}. However $E_{l+1,l+1}$ does not meet the traceless condition (5-120) and thus is not an infinitesimal operator of SU_n. To remedy this shortcoming, we take a suitable linear combination of the operators $E_{11}, \ldots, E_{ll}$ and $E_{l+1,l+1}$ to obtain a traceless operator. We usually put it in the form,

$$H_l = \frac{1}{l+1}\left(\sum_{i=1}^{l} E_{ii} - l E_{l+1,l+1}\right) = \frac{1}{l+1}\left(\sum_{i=1}^{l} \hat{n}_i - l\hat{n}_{l+1}\right) , \quad l = n-1, \ldots, 1 , \tag{7-51}$$

where (7-15) has been used.

The H_l obviously commute with one another and with the invariants $I'^{(m)}_k$ of $SU_m (m = n, n-1, \ldots, 2)$, since from (7-20) it is known that acting on any f–particle product state the operator $I'^{(m)}_k$ will not change the particle number in any single particle state.

The CSCO of the subgroup chain (7-49) and its corresponding intrinsic subgroup chain are

$$C(s) = \left(\{I'^{(n-1)}_k\}\ ,\ldots, I'^{(2)}_2;\ H_{n-1},\ldots,H_2,H_1\right)\ . \tag{7-52a}$$

$$\overline{C}(s) = \left(\{\overline{I}'^{(n-1)}_k\}\ ,\ldots, \overline{I}'^{(2)}_2;\ \overline{H}_{n-1},\ldots,\overline{H}_2,\overline{H}_1\right)\ , \tag{7-52b}$$

each consisting of $\frac{1}{2}n(n-1)$ operators. Equation (7-50), together with (7-52) provide $r = n^2-1$ operators which form the CSCO–III, $K = \left(C, C(s), \overline{C}(s)\right)$, of the group SU_n, while $\left(C, C(s)\right)$ forms the CSCO–II of SU_n.

Example 1: The group SU_2. The spin–up and spin–down states $\varphi_{1/2}$ and $\varphi_{-1/2}$ carry the fundamental rep of SU_2. The generators of SU_2 are the Pauli matrices σ_x, σ_y and σ_z [Eq. (7-39b)]. The CSCO–I of SU_2 consists of a single operator $I'^{(2)}$. From (7-19), (7-20) and (7-39b) we find

$$I'^{(2)} = 2\mathbf{J}^2 = 2(J_x^2 + J_y^2 + J_z^2)\ , \tag{7-53}$$

where $\mathbf{J} = \frac{1}{2}\boldsymbol{\sigma}$.

The irreps of SU_2 can be labelled either by the partitions $[\nu] = [m_{12}, m_{22}]$ or by the eigenvalues of $J^2 = \frac{1}{2}I'^{(2)}$. From (7-21) and (7-38c) we have

$$\mathbf{J}^2 = \tfrac{1}{2}(m_{12}-m_{22})\left[\tfrac{1}{2}(m_{12}-m_{22})+1\right]\ .$$

Since $\mathbf{J}^2 = J(J+1)$, we get a relation between J and the partition $[\nu] = [m_{12}, m_{22}]$,

$$J = \tfrac{1}{2}(m_{12}-m_{22})\ . \tag{7-54a}$$

We generally use J instead of $J(J+1)$ to label the SU_2 irreps. The partition $[\nu] = [m_{12}, m_{22}]$ can be expressed in terms of J and the particle number $f = m_{12} + m_{22}$ as

$$[\nu] = \left[\tfrac{f}{2}+J, \tfrac{f}{2}-J\right]\ . \tag{7-54b}$$

The meaning of (7-54) will be seen more clearly in Eq. (7-72b). The conjugate partition $[\tilde{\nu}]$ is

$$[\tilde{\nu}] = \left[2^{\frac{f}{2}-J}1^{2J}\right]\ . \tag{7-54b}$$

A canonical group chain of SU_2 is $SU_2 \supset U_1$. The CSCO–II and CSCO–III of SU_2 are (J^2, J_z) and $(J^2, J_z, \overline{J}_z)$, respectively (see Chapter 5).

Example 2: The group SU_3. The three flavor quarks u, d, and s carry the fundamental rep of SU_3, while $(u,d), (d,s)$ and (s,u) carry the fundamental reps of the three kinds of SU_2 subgroups, corresponding to the I–, U– and V–spin reps, respectively. A canonical group chain of SU_3 is $SU_3 \supset SU_2 \times U_1 \supset SO_2$. The eight generators of SU_3 are given in (5-110) and (5-123). The CSCO–I of SU_3 is $C = (I'^{(3)}_3, I'^{(2)}_2)$. The CSCO–I of SU_2 and SO_2 are taken as the isospin I^2 and its projection I_z, that for U_1 is chosen as the hypercharge

$$Y = \tfrac{1}{3}(E_{11} + E_{22} - 2E_{33})\ ,$$

which is identical to H_2 in (7-51). The physical meaning of the hypercharge will be seen in (7-72c). For SU_3 its CSCO–II is

$$\left(C; C(s)\right) = \left(I'^{(3)}_3,\ I'^{(3)}_2;\ I^2,\ I_z\ , Y\right)\ . \tag{7-55a}$$

The irreducible bases of SU_3 are eigenfunctions of the CSCO–II and are labelled by the five quantum numbers $(pq)II_zY$,

$$\begin{pmatrix} I'^{(3)}_3 \\ I'^{(3)}_2 \\ I^2 \\ I_z \\ Y \end{pmatrix} \psi^{(pq)}_{II_zY} = \begin{pmatrix} p \\ q \\ I(I+1) \\ I_z \\ Y \end{pmatrix} \psi^{(pq)}_{II_zY}\ . \tag{7-55b}$$

We will show in (7-71) that the irrep of SU_3 can be labelled by the partition $[\nu] = [m_{13}, m_{23}]$. It was shown in Sec. 5.24.2 that to label irreps of SU_3 we only need to use two integers (a_1, a_2), or (λ, μ), which are related to the partition $[\nu]$ by $\lambda = m_{13} - m_{23}$ and $\mu = m_{23}$ [see (5-357d)]. The eigenvalues p and q of the CSCO–I of SU_3 are functions of λ and μ. For example, from (7-38c) and (7-21), and noting that the particle number $f = m_{13} + m_{23} = \lambda + 2\mu$, we obtain [compare this with Eq. (5-304c)],

$$q = 2\left[\tfrac{1}{3}(\lambda - \mu)^2 + \lambda + \mu + \lambda\mu\right] . \tag{7-55c}$$

Later we will use $\psi^{(\lambda\mu)}_{II_zY}$ to denote an irreducible basis of SU_3.

The CSCO–III of SU_3 consists of the eight operators

$$K = (C, C(s), \overline{C}(s)) = (I'^{(3)}_3, I'^{(3)}_2, I^2, I_z, Y, \overline{I}^2, \overline{I}_z, \overline{Y}) . \tag{7-55d}$$

The complex conjugates of the common eigenfunctions of K in the group–parameter space yield the irreducible matrix elements of SU_3,

$$D^{(pq)}_{II_zY,\overline{II}_z\overline{Y}}(a^1 a^2 \ldots a^8) , \tag{7-55e}$$

where $a^1, \ldots, a^8$ are group parameters. For further discussion of the irreducible matrices of SU_3, readers are referred to Akyemapong (1972).

7.4. The Gel'fand Basis and Gel'fand Matrix Elements

The $U_n \supset U_{n-1} \supset \ldots \supset U_2 \supset U_1$ (or $SU_n \supset SU_{n-1} \times U_1 \supset \ldots \supset SU_2 \times U_1$) irreducible bases are referred to as the *Gel'fand bases* of $U_n(SU_n)$ (Gel'fand 1950, Baird 1963), which are usually labelled by the Gel'fand tableaux,

$$\left| \begin{pmatrix} [\nu] \\ (m) \end{pmatrix} \right\rangle = \left| \begin{pmatrix} m_{1n} & m_{2n} & \cdots & \cdots & m_{nn} \\ & m_{1n-1} & \cdots & m_{n-1n-1} & \\ & & \cdots\cdots & & \\ & & m_{12} m_{22} & & \\ & & m_{11} & & \end{pmatrix} \right\rangle , \tag{7-56}$$

with $[\nu] = [m_{11} m_{12} \ldots m_{nn}]$. For $SU_n, m_{nn} = 0$, [see (7-71)]. Equation (7-56) belongs to the irrep $[m_{1\ell} m_{2\ell} \ldots m_{\ell\ell}]$ of $U_\ell, \ell = n, n-1, \ldots 1$. m_{ij} are positive integers and obey the "betweenness condition"

$$m_{i,j+1} \geq m_{i+1,j+1} \geq m_{ij}$$

The Gel'fand basis functions are eigenfunctions of the CSCO–II $(C, C(s))$ of U_n [see Eqs. (7-46) and (7-47)].

We can define a so–called lexical ordering for the Gel'fand basis vectors by considering a Gel'fand tableau as a vector,

$$\mathbf{m} = (m_{1n} \ldots m_{nn}, m_{1n-1} \ldots m_{n-1n-1}, \ldots m_{12}, m_{22}, m_{11}) .$$

We shall say that the basic vector $\left|\binom{[\nu]}{(m)}\right\rangle$ precedes the vector $\left|\binom{[\nu]}{(m')}\right\rangle$, if the first non–vanishing component of the vector $\mathbf{m} - \mathbf{m}'$ is positive. For example, see Table 7.5-2.

The matrix elements of the infinitesimal operators $E_{n,n-1}$ of the group U_n in the Gel'fand basis were first given by Gel'fand (1950), and re-derived by Baird (1963). For example

$$E_{21} \begin{pmatrix} m_{12} & & m_{22} \\ & m_{11} & \end{pmatrix} = [(m_{11} - m_{22})(m_{12} - m_{11} + 1)]^{1/2} \begin{pmatrix} m_{12} & m_{22} \\ m_{11} - 1 & \end{pmatrix} , \tag{7-57}$$

$$E_{32}\begin{pmatrix} m_{13} & m_{23} & m_{33} \\ & m_{12} \quad m_{22} & \\ & m_{11} & \end{pmatrix}$$
$$= \left[\frac{m_{11}-m_{12}}{m_{22}-m_{12}-1}\right]^{\frac{1}{2}}\left[(-)\frac{(m_{13}-m_{12}+1)(m_{23}-m_{12})(m_{33}-m_{12}-1)}{(m_{22}-m_{12})}\right]^{\frac{1}{2}}\begin{pmatrix} m_{13} & m_{23} & m_{33} \\ & m_{12}-1, \quad m_{22} & \\ & m_{11} & \end{pmatrix}$$
$$+\left[\frac{m_{11}-m_{22}+1}{m_{12}-m_{22}+1}\right]^{\frac{1}{2}}\left[(-)\frac{(m_{13}-m_{22}+2)(m_{23}-m_{22}+1)(m_{33}-m_{22})}{(m_{12}-m_{22}+2)}\right]^{\frac{1}{2}}\begin{pmatrix} m_{13} & m_{23} & m_{33} \\ & m_{12}, \quad m_{22}-1 & \\ & m_{11} & \end{pmatrix}. \tag{7-58}$$

Using (7-11), from the matrices of the adjacent infinitesimal operators $E_{i,i-1}$, we can obtain matrices for the non-adjacent infinitesimal operators.

The formula for the Gel'fand matrix elements of the operator $E_{n,n-1}$ become very cumbersome for large n. Paldus (1974) gave a simplified formula for the two-column irreps encountered in the many-electron problem, while Kent and Schlesinger (1989, 1997) calculated the multi-body operator matrix elements in Gel'fand bases by using a graphical approach.

The Gel'fand basis is widely used due to the following attractive features:

1. It is an orthonormal basis

$$\left\langle \begin{pmatrix} [\nu'] \\ (m') \end{pmatrix} \middle| \begin{pmatrix} [\nu] \\ (m) \end{pmatrix} \right\rangle = \delta_{\nu\nu'}\delta_{(m)(m')} .$$

2. It is multiplicity free, since $U_n \supset U_{n-1} \supset \ldots \supset U_2 \supset U_1$ is a canonical group chain. In other words, a basis vector is uniquely labelled by a Gel'fand tableau.

3. In this basis, the matrix elements of the infinitesimal operator of U_n have algebraic formulas.

4. It is closely related to the Yamanouchi basis of the permutation group. As will be seen, the Gel'fand bases for unitary groups are quasi-standard bases of the permutation group.

Nevertheless, it also suffers from a serious drawback, namely, more often then not, it is not the basis we need in physics, except in some rare cases (for example in the quark model of elementary particles; for details see Sec. 7.5).

Ex. 7.1. Using (7-57) show that the representation matrix of $E_{32}E_{23}$ in the basis $\left\{\left|\begin{pmatrix} 2 & 1 & 0 \\ & 2 & 0 \\ & & 1 \end{pmatrix}\right\rangle, \left|\begin{pmatrix} 2 & 1 & 0 \\ & 1 & 1 \\ & & 1 \end{pmatrix}\right\rangle\right\}$ is equal to $I + D^{[21]}(23)$, where I is a unit matrix and $D^{[21]}(23)$ is the irreducible matrix for the permutation p_{23}.

Ex. 7.2. Using $E_{13} = [E_{12}, E_{23}]$ calculate $E_{13}\left|\begin{pmatrix} 2 & 1 & 0 \\ & 1 & 1 \\ & & 1 \end{pmatrix}\right\rangle$.

7.5. The Gel'fand Basis of Unitary Groups and the Quasi-Standard Basis of Permutation Groups

7.5.1. The CSCO-II of unitary groups and CSCO of the broken chains of permutation groups

We now proceed to extend (7-37) to the more general expression involving the invariants of subgroups of $\mathcal{U}_n$ and the class operators of subgroups of $\mathcal{S}_f$. We still consider the configuration $(m_1)^{f_1}(m_2)^{f_2}\ldots(m_n)^{f_n}$ with $\sum_{i=1}^{n} f_i = f$.

We define the following operator in analogy to (7-31)

$$P_k^{(f-f_n)} = \binom{f-f_n}{k}^{-1} \frac{1}{k!} \sum_{a_1>a_2>\ldots>a_k=1}^{f} \sum_{i_1 i_2 \ldots i_k=1}^{n-1} (e_{i_1 i_2}^{(a_1)} e_{i_2 i_3}^{(a_2)} \ldots e_{i_k i_1}^{(a_k)})_s \ . \tag{7-59}$$

Applying $P_k^{(f-f_n)}$ to the normal order state

$$|\omega\rangle = |\overbrace{m_1 \ldots m_1}^{f_1} \overbrace{m_2 \ldots m_2}^{f_2} \ldots \overbrace{m_n \ldots m_n}^{f_n}\rangle \ , \tag{7-60}$$

and using (5-94c), we get

$$\begin{aligned} P_k^{(f-f_n)}|\omega\rangle &= \binom{f-f_n}{k}^{-1} \frac{1}{k!} \sum_{a_1>a_2>\ldots>a_k=1}^{f-f_n} (a_1 a_2 \ldots a_k)_s |\omega\rangle \\ &= \frac{1}{g_k'} \sum_{a_1>a_2>\ldots>a_k=1}^{f-f_n} (a_1 (a_2 \ldots a_k)_s)|\omega\rangle \\ &= \frac{1}{g_k'} C_{(k)}(f-f_n)|\omega\rangle = \frac{1}{g_k'} \mathcal{C}_{(k)}(f-f_n)|\omega\rangle \\ &= \mathcal{C}^{(k)}(f-f_n)|\omega\rangle \end{aligned} \tag{7-61}$$

where (3-110) has been used in the last step, and $g_k' = \binom{f-f_n}{k}(k-1)!$ [see (1-23)], and $C_{(k)}(f-f_n)$ is the k–cycle class operator of the group $S_{f-f_n}(1,2,\ldots,f-f_n)$, while $\mathcal{C}^{(k)}(f-f_n)$ is the average k–cycle class operator of the state permutation group $\mathcal{S}_{f-f_n}(i_1 i_2 \ldots i_{f-f_n})$.

Similarly we can prove that acting on a non–normal ordered state

$$|\tilde{\omega}\rangle = p|\omega\rangle = \begin{pmatrix} 1 & 2 & \ldots & f \\ p_1 & p_2 & \ldots & p_f \end{pmatrix} |\omega\rangle \tag{7-62}$$

$P_k^{(f-f_n)}$ gives

$$\begin{aligned} P_k^{f-f_n}|\tilde{\omega}\rangle &= \binom{f-f_n}{k}^{-1} \frac{1}{k!} \sum_{a_1>a_2>\ldots>a_k}{}' (a_1 a_2 \ldots a_k)_s |\tilde{\omega}\rangle \\ &= \frac{1}{g_k'} C_{(k)}(f-f_n)'|\tilde{\omega}\rangle = \mathcal{C}^{(k)}(f-f_n)|\tilde{\omega}\rangle, \end{aligned} \tag{7-63}$$

where the prime in the summation symbol means that the indices $a_1, a_2, \ldots, a_k$ are to be taken from among the indices $p_1, p_2, \ldots, p_{f-f_n}$, and $C_{(k)}(f-f_n)'$ is the k–cycle class operator of the permutation group $S_{f-f_n}(p_1, p_2 \ldots, p_{f-f_n})$. For example, for $n=3, f=6, f_n=2$,

$$\begin{gathered} |\omega\rangle = |m_1 m_1 m_2 m_2 m_3 m_3\rangle \ , \ p = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 6 & 2 & 1 & 5 & 3 & 4 \end{pmatrix} \ , \\ |\tilde{\omega}\rangle = p|\omega\rangle = |m_2 m_1 m_3 m_3 m_2 m_1\rangle \ . \end{gathered}$$

From (7-59) and (7-4) we have

$$\begin{aligned} P_2^4|\tilde{\omega}\rangle &= \left(\frac{1}{6} \sum_{a_1>a_2=1}^{6} \sum_{i_1 i_2=m_1}^{m_2} e_{i_1 i_2}^{(a_1)} e_{i_2 i_1}^{(a_2)} \right) (\varphi_{m_2}^{(1)} \varphi_{m_1}^{(2)} \varphi_{m_3}^{(3)} \varphi_{m_3}^{(4)} \varphi_{m_2}^{(5)} \varphi_{m_1}^{(6)}) \\ &= \frac{1}{6}[(12)+(15)+(16)+(25)+(26)+(56)]|\tilde{\omega}\rangle \\ &= \frac{1}{6} C_{(2)}(4)'|\tilde{\omega}\rangle = \frac{1}{6} \mathcal{C}_{(2)}(4)|\tilde{\omega}\rangle \end{aligned}$$

where $C_{(2)}(4)'$ is the two-cycle class operator of $S_4(1256)$. Therefore, acting on any state $p|\omega\rangle$, the operator $P_k^{f-f_n}$ is always equivalent to the average k-cycle class operator $C^{(k)}(f-f_n)$ of the state permutation group $\mathcal{S}_{f-f_n}$. On the other hand, in analogy with (7-31) and (7-33), $P_k^{f-f_n}$ can be expressed in terms of the invariants $\Im_k^{(n-1)},\ldots,\Im_2^{(n-1)}$ and $\Im_1^{(n-1)}$ of the group $\mathcal{U}_{n-1}$. Thus $\Im_k^{(n-1)}$ can be expressed in terms of the class operators $\mathcal{C}_{(k)}(f-f_n),\ldots,\mathcal{C}_{(2)}(f-f_n)$ of $\mathcal{S}_{f-f_n}$, that is, in terms of the CSCO-I of $\mathcal{S}_{f-f_n}$,

$$\Im_k^{(n-1)} = F_k^{(n-1)}(\mathcal{C}(f-f_n)) \,. \tag{7-64a}$$

In the same way, we can prove that

$$\begin{aligned} &\Im_k^{(n-2)} = F_k^{(n-2)}(\mathcal{C}(f-f_n-f_{n-1})) \,, \\ &\cdots \\ &\Im_k^{(2)} = F_k^{(2)}(\mathcal{C}(f_1+f_2)) \,, \\ &\Im^{(1)} = f \,. \end{aligned} \tag{7-64b}$$

According to Sec. 4.8, the quasi-standard basis vectors $\psi^{(\nu)}$ are eigenfunctions of the operator set $(\mathcal{C}(f),\mathcal{C}(f-f_n),\ldots,\mathcal{C}(f_1+f_2),\mathcal{C}(f_1))$, the CSCO of the broken chain $\mathcal{S}_f \supset \mathcal{S}_{f-f_n} \supset \ldots \supset \mathcal{S}_{f_1+f_2} \supset \mathcal{S}_{f_1}$. From (7-37) and (7-64) it is seen that the quasi-standard basis vectors $\psi^{(\nu)\kappa}$ are eigenfunctions of the CSCO-II of $\mathcal{U}_n$. Therefore we have the following theorem.

Theorem 7.2: The quasi-standard basis of the permutation group is the Gel'fand basis of the unitary group.

Since the Yamanouchi basis is a special case of the quasi-standard basis, the Yamanouchi basis is also a Gel'fand basis of the unitary group. For example

$$|Y_m^{[\nu]}\rangle = \left|\begin{array}{|c|c|c|}\hline \alpha & \beta & \delta \\ \hline \gamma \\ \cline{1-1}\end{array}\right\rangle = \left|\begin{pmatrix} 3 & 1 & 0 & 0 \\ & 2 & 1 & 0 \\ & & 2 & 0 \\ & & & 1 \end{pmatrix}\right\rangle = \left|\begin{pmatrix}[\nu] \\ (m)\end{pmatrix}\right\rangle \,. \tag{7-65}$$

Based on the above facts, we immediately obtain from (7-40) the relation between the Yamanouchi matrix elements $D^{[\nu]}_{m'm}(ij)$ of the permutation group and Gel'fand matrix elements of the unitary group:

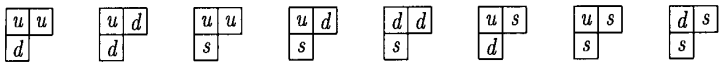
$$D^{[\nu]}_{m'm}(ij) = \sum_{(m'')} \left\langle \begin{pmatrix}[\nu] \\ (m')\end{pmatrix} \middle| E_{ij} \middle| \begin{pmatrix}[\nu] \\ (m'')\end{pmatrix} \right\rangle \left\langle \begin{pmatrix}[\nu] \\ (m)\end{pmatrix} \middle| E_{ij} \middle| \begin{pmatrix}[\nu] \\ (m'')\end{pmatrix} \right\rangle - \delta_{m'm} \,. \tag{7-66}$$

From (7-66) we also know that the Yamanouchi phase convention that the off-diagonal matrix elements $D^{[\nu]}_{m'm}(i,i-1)$ be positive is consistent with the *Gel'fand-Biedenharn phase convention* of the unitary group that the matrix elements of $E_{i,i-1}$ be positive.

7.5.2. The labelling and finding of the Gel'fand basis

The Weyl tableaux used to label the quasi-standard basis of the state-permutation group in Chapter 4 can now be used to label the Gel'fand basis of the unitary group. In view of the one-to-one correspondence between the Weyl tableau and Gel'fand symbol (see Sec. 4.8), the dimension $h_\nu(\mathcal{U}_n)$ of an irrep $[\nu]$ of $\mathcal{U}_n$ can be decided upon by counting the total allowed Weyl tableaux associated with the given partition $[\nu]$. So $h_\nu(\mathcal{U}_n)$ is equal to the total number of different Weyl tableaux filled with the n single particle states $m_1, m_2, \ldots, m_n$. For example, for

$n = 3, m_1 = u, m_2 = d, m_3 = s$, according to the rule for writing Weyl tableaux, we obtain the eight Weyl tableaux associated with the partition [21] as follows



(7-67)

Therefore the dimension of the irrep [21] of $\mathcal{SU}_3$ is $h_{[21]}(\mathcal{SU}_3) = 8$.

From Sec. 4.8 we know that when two identical state indices appear in the same column of a Weyl tableau $W_k^{[\nu]}$, the Gel'fand basis vector $|W_k^{[\nu]}\rangle = 0$. Consequently, the Young diagram of $\mathcal{U}_n$ or $\mathcal{SU}_n$ can have at most only n rows.

A formula for the dimensionality of $\mathcal{SU}_n$ irreps is as follows (Hamermesh 1962)

$$h_{[\nu]}(\mathcal{U}_n) = \prod_{1 \le i < j \le n} \frac{(\nu_i - i - \nu_j + j)}{j - i} \,. \tag{7-68a}$$

Thus for instance, the dimension for the irrep $(\lambda\mu)$ of SU_3

$$h_{(\lambda\mu)} = \tfrac{1}{2}(\lambda + 1)(\mu + 1)(\lambda + \mu + 2) \,. \tag{7-68b}$$

and the dimensions for the symmetric rep $[r]$ and antisymmetric rep $[1^r]$ of $\mathcal{SU}_n$ are

$$h_{[r]}(\mathcal{U}_n) = \binom{n + r - 1}{r} \,, \quad h_{[1^r]}(\mathcal{U}_n) = \binom{n}{r} \,. \tag{7-68c}$$

A simple formula was given by Robinson (1961). For example we have

$$h_{[422]}(\mathcal{U}_n) = \begin{array}{|c|c|c|c|} \hline n & n+1 & n+2 & n+3 \\ \hline n-1 & n & \multicolumn{2}{c}{} \\ \cline{1-2} n-2 & n-1 & \multicolumn{2}{c}{} \\ \cline{1-2} \end{array} \Big/ \begin{array}{|c|c|c|c|} \hline 6 & 5 & 2 & 1 \\ \hline 3 & 2 & \multicolumn{2}{c}{} \\ \cline{1-2} 2 & 1 & \multicolumn{2}{c}{} \\ \cline{1-2} \end{array}$$

$$= \frac{n^2(n+1)(n+2)(n+3)(n-1)(n-2)(n-1)}{6 \cdot 5 \cdot 2 \cdot 1 \cdot 3 \cdot 2 \cdot 2 \cdot 1} \,, \tag{7-69}$$

where the denominator is the product of the hook lengths defined in (4-4b), while the numerator is a product of integers. The rule for filling the integers in a Young diagram is as follows: Fill all the boxes along the diagonal of the Young diagram with the integer n, and fill consecutively the subsequent boxes in the rows with $n+1, n+2$, and so on, and in the same columns with $n-1, n-2$, and so on. The dimension of the adjoint rep $[21^{n-2}]$ of $\mathcal{SU}_n$ is easily found to be $n^2 - 1$ by Robinson's formula,

$$h_{[21^{n-2}]}(\mathcal{SU}_n) = \begin{array}{|c|c|} \hline n & n+1 \\ \hline n-1 & \multicolumn{1}{c}{} \\ \cline{1-1} \vdots & \multicolumn{1}{c}{} \\ \cline{1-1} 3 & \multicolumn{1}{c}{} \\ \cline{1-1} 2 & \multicolumn{1}{c}{} \\ \cline{1-1} \end{array} \Big/ \begin{array}{|c|c|} \hline n & 1 \\ \hline n-2 & \multicolumn{1}{c}{} \\ \cline{1-1} \vdots & \multicolumn{1}{c}{} \\ \cline{1-1} 2 & \multicolumn{1}{c}{} \\ \cline{1-1} 1 & \multicolumn{1}{c}{} \\ \cline{1-1} \end{array} = \frac{(n+1)!}{n \times (n-2)!} = n^2 - 1 \,.$$

$\mathcal{SU}_n$ is a simple group and has $n^2 - 1$ infinitesimal operators, which carry the adjoint rep $[21^{n-2}]$ of $\mathcal{SU}_n$.

Now we turn to study the transformation property of the totally anti-symmetric state $[1^n]$

under group elements $\mathcal{R}$ of $\mathcal{U}_n$.

$$\mathcal{R}\left|\begin{array}{|c|}\hline m_1\\\hline m_2\\\hline \vdots\\\hline m_n\\\hline\end{array}\right\rangle = \mathcal{R}\left[\frac{1}{\sqrt{n!}}\sum_{m_1\ldots m_n}\varepsilon_{m_1\ldots m_n}\varphi^{a_1}_{m_1}\ldots\varphi^{a_n}_{m_n}\right] \tag{7-70a}$$

$$= \frac{1}{\sqrt{n!}}\sum_{\substack{m_1\ldots m_n\\ m'_1\ldots m'_n}}\varepsilon_{m_1\ldots m_n}\mathcal{D}_{m'_1 m_1}\ldots\mathcal{D}_{m'_n m_n}\varphi^{a_1}_{m'_1}\ldots\varphi^{a_n}_{m'_n}$$

$$= \det(\mathcal{D})|[1^n]\rangle = e^{i\varphi}|[1^n]\rangle$$

where (5-72b) and the following expression for the determinant $\det(\mathcal{D})$ has been used,

$$\det(\mathcal{D}) = \sum_{i_1\ldots i_n}\varepsilon^{i_1\ldots i_n}\varepsilon^{i'_1\ldots i'_n}\mathcal{D}_{i'_1 i_1}\ldots\mathcal{D}_{i'_n i_n}\ . \tag{7-70b}$$

Analogously we can show that

$$\mathcal{R}|[m^n]\rangle = e^{im\varphi}|[m^n]\rangle\ . \tag{7-70c}$$

Suppose that the group $\mathcal{U}_n$ has an irrep $[\nu] = [\nu_1\nu_2\ldots\nu_n]$. Annexing a single column of n boxes to the Young diagram $[\nu]$ gives a new representation $[\nu'] = [\nu_1+1, \nu_2+1, \ldots, \nu_n+1]$. Obviously, the irreps $[\nu]$ and $[\nu']$ of $\mathcal{U}_n$ have the same number of Weyl tableaux and thus have the same dimension. From (7-70a) it is known that the only change in the representation matrices due to the annexing is that they are multiplied by a common factor $e^{i\varphi}$. Similarly, the irreps $[\nu'] = [\nu_1+m, \nu_2+m, \ldots, \nu_n+m]$ and $[\nu]$ of $\mathcal{U}_n$ have the same dimension and their representation matrices differ only by a common factor $e^{im\varphi}$, that is,

$$D^{[\nu_1\nu_2\ldots]}(\mathcal{U}_n) = e^{-im\varphi}D^{[\nu_1+m,\nu_2+m,\ldots]}(\mathcal{U}_n)\ . \tag{7-70d}$$

If we are dealing with the special unitary group $\mathcal{SU}_n, \det(\mathcal{D}) = e^{i\varphi} = 1$, and we have

$$D^{[\nu_1\nu_2\ldots]}(\mathcal{SU}_n) = D^{[\nu_1+m,\nu_2+m\ldots]}(\mathcal{SU}_n)\ . \tag{7-70e}$$

Therefore for the group $\mathcal{SU}_n$, the irreps $[\nu_1\ldots\nu_n]$ and $[\nu_1+m, \ldots, \nu_n+m]$ are equivalent, and we only need consider those Young diagrams which have at most $n-1$ rows:

$$[\nu_1\nu_2\ldots\nu_n] \equiv [\nu_1-\nu_n, \nu_2-\nu_n, \ldots, \nu_{n-1}-\nu_n, 0] \tag{7-71}$$

and the irrep $[1^n]$ or $[m^n]$ becomes the identity rep designated as $[0]$.

In atomic or nuclear physics, the state belonging to the irrep $[1^n]$ corresponds to a closed shell state. Under the group $\mathcal{SU}_n$, it behaves, like a vacuum state and thus can be ignored.

We can use the three labelling schemes for the quasi-standard basis of the permutation group to characterize the Gel'fand basis, since these two bases are identical. We often use other quantum numbers to label the Gel'fand basis anyway. For example, for the group $\mathcal{SU}_2$, we often use the quantum numbers J and J_z, which are related to the Gel'fand symbol by

$$J = \frac{1}{2}(m_{12}-m_{22})\ ,\quad J_z = m_{11}-\frac{1}{2}(m_{12}+m_{22})\ . \tag{7-72a}$$

The first equation is just equation (7-54). We can easily use the Weyl tableaux to derive (7-72a). Let us fill the boxes in the first row of a Young diagram $[m_{12}m_{22}]$ with the spin up states α, and the second row with the spin down states β. The state corresponding to this Weyl tableau

has the maximum possible J_z value for the irrep $[m_{12}, m_{22}]$, that is, $J_z = \frac{1}{2}(m_{12} - m_{22})$. Thus the total spin must be $J = \frac{1}{2}(m_{12} - m_{22})$.

A general Weyl tableau corresponding to the Gel'fand symbol $\begin{pmatrix} m_{12} & m_{22} \\ & m_{11} \end{pmatrix}$ is as follows.

$$\begin{pmatrix} m_{12} & m_{22} \\ & m_{11} \end{pmatrix} = \begin{array}{|c|c|} \hline m_{11}\alpha\text{'s} & (m_{12}-m_{11})\beta\text{'s} \\ \hline m_{22}\beta\text{'s} \\ \cline{1-1} \end{array} \quad . \tag{7-72b}$$

The corresponding state has $J = \frac{1}{2}(m_{12} - m_{22})$ and

$$J_z = \frac{1}{2}[m_{11} - (m_{12} - m_{11} + m_{22})] = m_{11} - \frac{1}{2}(m_{12} + m_{22}) \ .$$

In the $\mathcal{SU}_4$ quark model of elementary particles, it is assumed that there exist four kinds of flavor quarks, u, d, s and c, carrying the fundamental rep of $\mathcal{SU}_4$. The quantum numbers of these flavor quarks are listed in Table 7.5-1. Q is the charge, I and I_z are the isospin and its z component, B, S, C and Y are the baryon number, strangeness, charm and hypercharge, respectively, while Z is a quantity introduced by Haacke (1976). I_z, Y and Z can be expressed in terms of the quark numbers n_u, n_d, n_s and n_c:

$$\begin{aligned} I_z &= \frac{1}{2}(n_u - n_d) \ , \\ Y = B + S &= \frac{1}{3}(n_u + n_d - 2n_s) \ , \quad \text{(only for } u, d, s\text{)} \\ Z &= \frac{1}{4}(n_u + n_d + n_s - 3n_c) \ . \end{aligned} \tag{7-72c}$$

Table 7.5-1. The quantum numbers of the flavor quarks u, d, s and c.

	Q	I	I_z	B	S	C	Y	Z
u	$\frac{2}{3}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{3}$	0	0	$\frac{1}{3}$	$\frac{1}{4}$
d	$-\frac{1}{3}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{3}$	0	0	$\frac{1}{3}$	$\frac{1}{4}$
s	$-\frac{1}{3}$	0	0	$\frac{1}{3}$	-1	0	$-\frac{2}{3}$	$\frac{1}{4}$
c	$\frac{2}{3}$	0	0	$\frac{1}{3}$	0	1	0	$-\frac{3}{4}$

We usually order the single quark states according to the sequence u, d, s and c, then I_z, Y and Z are the eigenvalues of the commuting operators H_1, H_2 and H_3 in (7-51).

The Gel'fand basis of SU_4 can be labelled in three ways: by a Gel'fand symbol, by a Weyl tableau, or by the quantum numbers $[\nu](\lambda\mu)IYZI_z$. Their mutual relations are given in (7-73).

$$\begin{pmatrix} m_{14} & m_{24} & m_{34} & 0 \\ m_{13} & m_{23} & m_{33} & \\ & m_{12} & m_{22} & \\ & & m_{11} & \end{pmatrix} \leftrightarrow \begin{array}{|l|} \hline m_{11}\text{ 1's, }(m_{12}-m_{11})\text{ 2's, }(m_{13}-m_{12})\text{ 3's, }(m_{14}-m_{13})\text{ 4's} \\ \hline m_{22}\text{ 2's, }(m_{23}-m_{22})\text{ 3's, }(m_{24}-m_{23})\text{ 4's} \\ \hline m_{33}\text{ 3's, }(m_{34}-m_{33})\text{ 4's} \\ \cline{1-1} \end{array} \tag{7-73}$$

Gel'fand basis Weyl tableau(1,2,3,4 denote the single quark states)

$$[\nu] = [m_{14}m_{24}m_{34}] , \qquad \lambda = (m_{13} - m_{23}) , \quad u = (m_{23} - m_{33}) ,$$
$$I = \frac{1}{2}(m_{12} - m_{22}) , \qquad I_z = m_{11} - \frac{1}{2}(m_{12} - m_{22})$$
$$Y = (m_{12} + m_{22}) - \frac{2}{3}(m_{13} + m_{23} + m_{33}) ,$$
$$Z = m_{13} + m_{23} + m_{33} - \frac{3}{4}(m_{14} + m_{24} + m_{34}) . \qquad (7\text{-}73b)$$

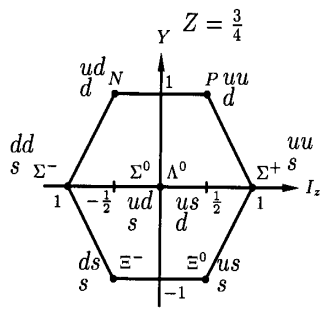
In elementary particle physics one often uses the dimensions to label irreps of $\mathcal{SU}_n$. For example, we use (20) to label the 20-dimensional irrep [21] of $\mathcal{SU}_4$, and (8) to label the 8-dimensional irrep [21] of $\mathcal{SU}_3$. Table A.1 in the Appendix gives the correspondence between dimensions and partitions of groups from SU_3-SU_6.

As an example, we list in Table 7.5-2 the three labelling schemes for the eight-dimensional irrep (the adjoint rep of $\mathcal{SU}_3$).

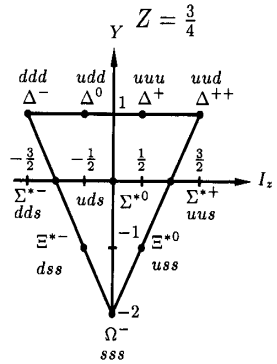
Table 7.5-2. Three labelling schemes for the eight-dimensional irrep of SU_3.

particles	P	N	Σ^+	Σ^0	Σ^-	Λ	Ξ^0	Ξ^-
(I, I_z, Y)	$(\frac{1}{2}\ \frac{1}{2},\ 1)$	$(\frac{1}{2}\ -\frac{1}{2},\ 1)$	(1 1, 0)	(1 0, 0)	(1 - 1, 0)	(0 0, 0)	$(\frac{1}{2}\ \frac{1}{2},\ -1)$	$(\frac{1}{2}\ -\frac{1}{2},\ -1)$
Weyl tableau	$\begin{array}{|c\|c\|}\hline u & u \\ \hline d \\ \cline{1-1}\end{array}$	$\begin{array}{|c\|c\|}\hline u & d \\ \hline d \\ \cline{1-1}\end{array}$	$\begin{array}{|c\|c\|}\hline u & u \\ \hline s \\ \cline{1-1}\end{array}$	$\begin{array}{|c\|c\|}\hline u & d \\ \hline s \\ \cline{1-1}\end{array}$	$\begin{array}{|c\|c\|}\hline d & d \\ \hline s \\ \cline{1-1}\end{array}$	$\begin{array}{|c\|c\|}\hline u & s \\ \hline d \\ \cline{1-1}\end{array}$	$\begin{array}{|c\|c\|}\hline u & s \\ \hline s \\ \cline{1-1}\end{array}$	$\begin{array}{|c\|c\|}\hline d & s \\ \hline s \\ \cline{1-1}\end{array}$
Gel'fand symbol	$\begin{pmatrix} 2\ 1\ 0 \\ 2\ 1 \\ 2 \end{pmatrix}$	$\begin{pmatrix} 2\ 1\ 0 \\ 2\ 1 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 2\ 1\ 0 \\ 2\ 0 \\ 2 \end{pmatrix}$	$\begin{pmatrix} 2\ 1\ 0 \\ 2\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 2\ 1\ 0 \\ 2\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 2\ 1\ 0 \\ 1\ 1 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 2\ 1\ 0 \\ 1\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 2\ 1\ 0 \\ 1\ 0 \\ 0 \end{pmatrix}$

In elementary particle physics, the $\mathcal{SU}_3$ irreducible basis vectors are usually plotted in the weight diagrams with the hypercharge Y as the y-axis and the third component I_z of the isospin as the x-axis (de Swart 1963). Figure 7.5-1 gives the weight diagrams for the irreps [21], [3] and $[1^3]$, with the dimensions 8, 10 and 1, respectively.



The baryon octet with $J^\pi = \frac{1}{2}^+$.



The baryon decuplet with $J^\pi = \frac{3}{2}^+$.

Fig.7.5-1. The weight diagrams of $\mathcal{SU}_3$ for the irreps [21], [3] and $[1^3]$.

The particles belonging to the same irrep of SU_3 form a multiplet and they should have the same baryon number, spin and parity. The baryon octet ($[\nu] = [21]$) and decuplet ($[\nu] = [3]$) have $J^\pi = \frac{1}{2}^+$ and $\frac{3}{2}^+$, respectively. Table 7.5-3 gives the masses of the members of the octet and decuplet. In the $\mathcal{SU}_3$ model, the strongest interactions are assumed to be invariant under $\mathcal{SU}_3$. In the absence of any other interactions, the members of the same multiplet should have

the same mass. The $\mathcal{SU}_3$ symmetry is broken by some unknown weaker interactions and the mass degeneracy of the particles belonging to the same unitary multiplet is removed, as is seen from Table 7.5-3. Okubo (1962) assumed that this symmetry-breaking interaction is due to the irreducible tensor $T^{[21]}_{000}$, that is, the $I = I_z = Y = 0$ component of the irrep [21] of $\mathcal{SU}_3$, and derived the following mass formulas, known as the *Gell-Mann–Okubo* mass formula (for the derivation see Lichtenberg 1978, p. 179),

$$\tfrac{1}{2}(M_N + M_\Xi) = \tfrac{3}{4}M_\Lambda + \tfrac{1}{4}M_\Sigma \ ,$$
$$M_{\Omega^-} - M_{\Xi^*} = M_{\Xi^*} - M_{\Sigma^*} = M_{\Sigma^*} - M_\Delta \ .$$

The Gell-Mann–Okubo formula works rather well for baryons.

Table 7.5-3. The masses of the members of the octet and decouplet (in MeV).

octet	P	N	Σ^+	Σ^0	Σ^-	Λ^0	Ξ^0	Ξ^-		
	938	940	1189	1192	1197	1116	1315	1321		
decuplet	Δ^{++}	Δ^+	Δ^0	Δ^-	Σ^{*+}	Σ^{*0}	Σ^{*-}	Ξ^{*0}	Ξ^{*-}	Ω^-
	1231	1231	1232	1239	1382	1381	1386	1532	1535	1672

If one further takes into account the electromagnetic interaction, which breaks the $\mathcal{SU}_2$ symmetry, then the masses of the different members of the same isomultiplet are split up. The SU_2 symmetry-breaking interaction is relatively minor, as is seen from Table 7.5-3 that the different members of an isomultiplet have masses which differ by less than 10 MeV.

The irrep [21] of $\mathcal{SU}_4$ is 20-dimensional. The weight diagrams of $\mathcal{SU}_4$ are three-dimensional with I_z, Y and Z as the coordinate axes. They can be resolved into plane diagrams according to the quantum number Z. For the irrep [21], the diagram with $Z = \frac{3}{4}$ is just the first diagram in Fig. 7.5-1, while those for $Z = -\frac{1}{4}$ and $-\frac{5}{4}$ are shown in Fig. 7.5-2.

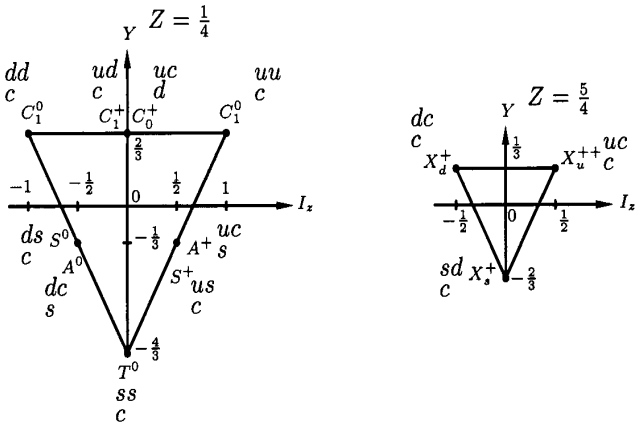


Fig. 7.5-2. The weight diagrams of $\mathcal{SU}_4$ for the irrep [21].

Now let us summarize the method of decomposing the reducible tensor (7-2) of U_n into the irreducible basis of $\mathcal{U}_n$ and S_f. With the notation used in Chapter 4, the reducible tensor (7-2) is expressed as

$$\Phi_a = p_a|\omega\rangle = p_a|i_1 i_2 \ldots i_f\rangle \ . \tag{7-74}$$

In the first place, according to the different configurations $(m_1)^{f_1}(m_2)^{f_2}\dots(m_n)^{f_n}$, the n^f basis vectors (7-74) are divided into several groups, and each group contains $\mathcal{N}_{f_1 f_2 \dots f_n}$ vectors where

$$\mathcal{N}_{f_1 f_2 \dots f_n} = f!/(f_1! f_2! \dots f_n!) , \tag{7-75a}$$

$$n^f = \sum_{f_1+f_2+\dots+f_n=f} \mathcal{N}_{f_1 f_2 \dots f_n} . \tag{7-75b}$$

Then for each configuration $(m_1)^{f_1}(m_2)^{f_2}\cdots(m_n)^{f_n}$, we proceed to reduce the $\mathcal{N}_{f_1 f_2 \dots f_n}$ basis vectors. Since the Gel'fand basis of the unitary group is the quasi-standard basis of the permutation group, the reduction problem for the unitary group is converted into that for the permutation group. Each irreducible basis vector resulting from the reduction of (7-74) is uniquely labelled by a Young tableau Y_m and a Weyl tableau W_κ:

$$\left| \begin{matrix}[\nu] \\ Y_m, W_\kappa \end{matrix} \right\rangle = \sum_{a=1}^{\mathcal{N}_{f_1 \dots f_n}} u_{\nu m \kappa, a} \Phi_a , \qquad \begin{matrix} m = 1, 2, \dots, h_\nu(S_f) \\ \kappa = 1, 2, \dots, \tau^\nu_{f_1 f_2 \dots f_n} \end{matrix} , \tag{7-76}$$

where $h_\nu(S_f)$ is the dimension of the irrep $[\nu]$ of S_f and $\tau^\nu_{f_1 \dots f_n}$ is the number of times the irrep $[\nu]$ of S_f occurs in the configuration $(m_1)^{f_1}(m_2)^{f_2}\dots(m_n)^{f_n}$. From the eigenequation (4-76) or (4-77), we can find the coefficients $u_{\nu m \kappa, a}$.

Under the action of the group S_f, (7-76) only changes its Young tableau Y_m,

$$p \left| \begin{matrix}[\nu] \\ Y_m, W_\kappa \end{matrix} \right\rangle = \sum_{m'=1}^{h_\nu(S_f)} D^{[\nu]}_{m'm}(p) \left| \begin{matrix}[\nu] \\ Y_{m'}, W_\kappa \end{matrix} \right\rangle , \tag{7-77a}$$

and under the action of the group $\mathcal{U}_n$, (7-76) only changes its Weyl tableau W_κ,

$$\mathcal{E}_{\alpha\beta} \left| \begin{matrix}[\nu] \\ Y_m, W_\kappa \end{matrix} \right\rangle = \sum_{\kappa'=1}^{h_\nu(\mathcal{U}_n)} \left\langle \begin{matrix}[\nu] \\ W_{\kappa'} \end{matrix} \middle| \mathcal{E}_{\alpha\beta} \middle| \begin{matrix}[\nu] \\ W_\kappa \end{matrix} \right\rangle \left| \begin{matrix}[\nu] \\ Y_m, W_{\kappa'} \end{matrix} \right\rangle , \tag{7-77b}$$

where $h_\nu(\mathcal{U}_n)$ is the dimension of the irrep $[\nu]$ of $\mathcal{U}_n$. The first factor on the right-hand side of (7-77b) is the Gel'fand matrix element. Obviously, the dimension $h_\nu(\mathcal{U}_n)$ is related to $\tau^\nu_{f_1 \dots f_n}$ by

$$h_\nu(\mathcal{U}_n) = \sum_{f_1+f_2+\dots+f_n=f} \tau^\nu_{f_1 f_2 \dots f_n} . \tag{7-78}$$

The total number of irreducible basis vectors is still n^f:

$$n^f = \sum_\nu h_\nu(S_f) h_\nu(\mathcal{U}_n) , \tag{7-79}$$

where the summation over ν includes all possible partitions $[\nu] = [\nu_1 \nu_2 \dots \nu_f]$ of the integer f.

The n^f irreducible basis vectors $\left| \begin{matrix}[\nu] \\ Y_m, W_\kappa \end{matrix} \right\rangle$ can be placed in a rectangular array in which the rows are labelled by Y_m and the columns by W_κ. The array is in block-diagonal form and consists of N blocks, N being the number of classes of S_f. Each block belongs to the irrep $[\nu]$ of S_f and $\mathcal{U}_n$. The basis vectors in any particular row of a block span the irrep $[\nu]$ of $\mathcal{U}_n$. There are $h_\nu(S_f)$ rows which indicates that the irrep $[\nu]$ of $\mathcal{U}_n$ occurs $h_\nu(S_f)$ times. Similarly, the basis vectors in each column of the block span the irrep $[\nu]$ of S_f. There are $h_\nu(\mathcal{U}_n)$ columns which implies that the irrep $[\nu]$ of S_f occurs $h_\nu(\mathcal{U}_n)$ times.

For example, suppose $f = 3$. The $3^3 = 27$ irreducible basis vectors of S_3 and $\mathcal{U}_3$ are placed in the rectangular array shown in Fig. 7.5-3.

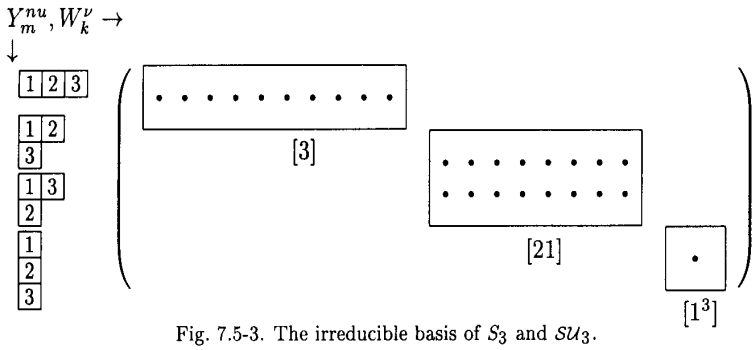


Fig. 7.5-3. The irreducible basis of S_3 and SU_3.
Note that $3^3 = 1 \times 10 + 2 \times 8 + 1 \times 1$. For the tableaux W_k^{ν}, see Fig. 7.5-1.

Table 7.5-4. The baryon SU_3 wave functions.

ν, m, k		$\|uds\rangle$	$\|dus\rangle$	$\|sdu\rangle$	$\|usd\rangle$	$\|sud\rangle$	$\|dsu\rangle$
3, 1, 1	$\|\boxed{1}\boxed{2}\boxed{3}, \Sigma^{*0}\rangle$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$
0, 1, 1	$\left\|\begin{smallmatrix}\boxed{1}\boxed{2}\\ \boxed{3}\end{smallmatrix}, \Sigma^0\right\rangle$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{3}}$	$-\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$
0, −1, 1	$\left\|\begin{smallmatrix}\boxed{1}\boxed{3}\\ \boxed{2}\end{smallmatrix}, \Sigma^0\right\rangle$	0	0	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$
0, 1, −1	$\left\|\begin{smallmatrix}\boxed{1}\boxed{2}\\ \boxed{3}\end{smallmatrix}, \Lambda^0\right\rangle$	0	0	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$
0, 1, 1	$\left\|\begin{smallmatrix}\boxed{1}\boxed{3}\\ \boxed{2}\end{smallmatrix}, \Lambda^0\right\rangle$	$\frac{1}{\sqrt{3}}$	$-\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{12}}$	$\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$
−3, −1, −1	$\left\|\begin{smallmatrix}\boxed{1}\\ \boxed{2}\\ \boxed{3}\end{smallmatrix}, [0]\right\rangle$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$

The explicit form of the 27 irreducible basis vectors of Fig. 7.5-3 was given in Chapter 3. By setting $\alpha = u, \beta = d$ and $\gamma = s$ in Table 3.9 and also by referring to Fig. 7.5-1 we obtain the wave functions of Σ^{*0}, Σ^0 and Λ^0 listed in Table 7.5-4.

By setting (α, β) in Table 3.4-1 equal to $(u, d), (u, s)$ and (d, s) respectively, from (3-90) we obtain the wave functions of the elementary particles P, Σ^+ and Σ^- listed in Table 7.5-5. Similarly, from Ex. 3.7 in Sec. 3.4, we obtain the wave functions of N, Ξ^0 and Ξ^- listed in Table 7.5-6.

The irreducible basis for the totally symmetric rep [3] is

$$\left| \boxed{1}\boxed{2}\boxed{3}\ \boxed{\alpha}\boxed{\alpha}\boxed{\beta} \right\rangle = \frac{1}{\sqrt{3}}\big(|\alpha\alpha\beta\rangle + |\alpha\beta\alpha\rangle + |\beta\alpha\alpha\rangle\big) \ . \tag{7-80}$$

The SU_4 baryon wave functions can be obtained from Table 7.5-4 by replacing the state labels (u, d, s) with (u, s, c) and (d, s, c), and from Table 7.5-5 and 7.5-6 by replacing (u, d) with $(u, c), (d, c)$ and (s, c).

In the above discussions, the coordinates of the f particles are assumed to be all different. If the coordinates of different particles are allowed to be identical, then the standard basis $\left| \begin{matrix}[\nu] \\ Y_m, W_\kappa \end{matrix} \right\rangle$ of S_f goes over to the quasi–standard basis $\left| \begin{matrix}[\nu] \\ W_m, W_\kappa \end{matrix} \right\rangle$ of S_f (or the Gel'fand basis of U_n), where W_m is the Weyl tableau in coordinate space. Under the action of the infinitesimal

Table 7.5-5. The baryon $\mathcal{SU}_3$ wave functions.

	$\|uud\rangle$	$\|udu\rangle$	$\|duu\rangle$
	$\|uus\rangle$	$\|usu\rangle$	$\|suu\rangle$
	$\|dds\rangle$	$\|dsd\rangle$	$\|sdd\rangle$
$\begin{array}{\|c\|c\|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}$; P, Σ^+, Σ^-	$\frac{2}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$
$\begin{array}{\|c\|c\|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}$; P, Σ^+, Σ^-	0	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$

Table 7.5-6

	$\|udd\rangle$	$\|dud\rangle$	$\|ddu\rangle$
	$\|uss\rangle$	$\|sus\rangle$	$\|ssu\rangle$
	$\|dss\rangle$	$\|sds\rangle$	$\|ssd\rangle$
$\begin{array}{\|c\|c\|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}$; N, Ξ^0, Ξ^-	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$-\frac{2}{\sqrt{6}}$
$\begin{array}{\|c\|c\|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}$; P, Ξ^0, Ξ^-	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0

operators E_{ij} and $\mathcal{E}_{\alpha\beta}$, the $[h_\nu(U_n)]^2$ irreducible basis vectors of U_n and $\mathcal{U}_n$ transform as follows:

$$E_{ij}\left|\begin{matrix}[\nu]\\ W_m, W_\kappa\end{matrix}\right\rangle = \sum_{m'=1}^{h_\nu(U_n)} \left\langle \begin{matrix}[\nu]\\ W_{m'}\end{matrix}\middle| E_{ij} \middle| \begin{matrix}[\nu]\\ W_m\end{matrix}\right\rangle \left|\begin{matrix}[\nu]\\ W_{m'}, W_\kappa\end{matrix}\right\rangle , \tag{7-81a}$$

$$\mathcal{E}_{\alpha\beta}\left|\begin{matrix}[\nu]\\ W_m, W_\kappa\end{matrix}\right\rangle = \sum_{\kappa'=1}^{h_\nu(U_n)} \left\langle \begin{matrix}[\nu]\\ W_{\kappa'}\end{matrix}\middle| \mathcal{E}_{\alpha\beta} \middle| \begin{matrix}[\nu]\\ W_\kappa\end{matrix}\right\rangle \left|\begin{matrix}[\nu]\\ W_m, W_{\kappa'}\end{matrix}\right\rangle . \tag{7-81b}$$

From (7-81) it is seen that as soon as any one of the $[h_\nu(U_n)]^2$ irreducible basis vectors is known, all the others can be found with the help of the Gel'fand matrix elements. However this method is not as simple as the EFM.

Starting with the next section, we will mainly be concerned with the unitary group in state space, and so we change our notation from $\mathcal{U}_n(\mathcal{SU}_n)$ to $U_n(SU_n)$ to be consistent with the conventional notation.

Ex. 7.3. For the irrep [3] of SU_3, construct the equivalent table to Table 7.5-2.

Ex. 7.4. Consider six quarks in the configuration $(u)^2(d)^2(s)^2$ and write out the possible Gel'fand basis vectors and their corresponding Gel'fand symbols.

7.6. The Contragredient Representation

According to Sec. 2.4 the rep $\widetilde{D}^{-1}$ is called the contragredient rep of D. If D is unitary, then $\widetilde{D}^{-1} = D^*$. It can be shown that the contragredient rep of the irrep $[\nu] = [\nu_1\nu_2\ldots\nu_n]$ is $[\nu'] = [\nu'_1, \nu'_2, \ldots, \nu'_n]$, where

$$\nu'_1 = \nu_1 - \nu_n\ , \quad \nu'_2 = \nu_1 - \nu_{n-1}, \ldots\ , \quad \nu'_p = \nu_1 - \nu_{n-p+1}, \ldots\ , \quad \nu'_n = 0\ . \tag{7-82}$$

The relation (7-82) is easily committed to memory by noting that putting the Young diagram $[\nu]$ and the upside down diagram of $[\nu']$ together, we get the Young diagram $[\nu_1^n]$, that is, the identity rep [0] of SU_n. For instance, corresponding to the irrep $[\nu] = [43221]$ of SU_5, the contragredient rep $[\nu'] = [3221]$, as shown in the Fig. 7.6-1.

A general proof of (7-82) is given by Elliott (1979). We will only discuss a special case of (7-82), where $[\nu] = [1]$, and $[\nu'] = [1^{n-1}]$.

Suppose $\varphi_{i_1}\ldots\varphi_{i_n}$ and $\psi^{i_1}\ldots\psi^{i_n}$ span the irreps [1] and $[1^{n-1}]$ of SU_n, respectively. The basis of the anti-symmetric rep $[1^{n-1}]$ can be expressed in terms of the determinant

$$\psi^{i_1} = \sum_{i_2\ldots i_n} \varepsilon^{i_1 i_2\ldots i_n}\varphi_{i_2}\ldots\varphi_{i_n}\ . \tag{7-83}$$

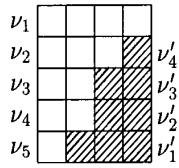


Fig. 7.6-1. The irrep $[\nu] = [43221]$ and its contragredient rep $[\nu'] = [3221]$ of SU_5.

Under the SU_n transformation

$$\begin{aligned}\psi^{i_1} \to \psi'^{i_1} &= \sum_{i_2 \ldots i_n} \sum_{i'_2 \ldots i'_n} \varepsilon^{i_1 i_2 \ldots i_n} \mathcal{D}_{i'_2 i_2} \ldots \mathcal{D}_{i'_n i_n} \varphi_{i'_2} \ldots \varphi_{i'_n} \\ &= \sum_{i'_2 \ldots i'_n} M_{i'_1 i_1} \varepsilon^{i'_1 i'_2 \ldots i'_n} \varphi_{i'_2} \ldots \varphi_{i'_n} \\ &= \sum_{i'_1} (\mathcal{D}^{-1})_{i_1 i'_1} \det(\mathcal{D}) \psi^{i'_1} = \sum_{i'_1} (\tilde{\mathcal{D}}^{-1})_{i'_1 i_1} \psi^{i'_1} \ , \end{aligned} \tag{7-84}$$

where $M_{i'_1 i_1}$ is the co–factor of the element $\mathcal{D}_{i'_1 i_1}$. In deriving (7-84) the following relations were used:

$$(\mathcal{D}^{-1})_{i_1 i'_1} = M_{i'_1 i_1} / \det(\mathcal{D}) \ , \tag{7-85a}$$

$$M_{i'_1 i_1} = \sum_{i_2 \ldots i_n} \varepsilon^{i_1 i_2 \ldots i_n} \varepsilon^{i'_1 i'_2 \ldots i'_n} \mathcal{D}_{i'_2 i_2} \ldots \mathcal{D}_{i'_n i_n} \ . \tag{7-85b}$$

Equation (7-84) shows that the basis $\psi^{i_1} \ldots \psi^{i_n}$ of the irrep $[1^{n-1}]$ of SU_n do transform according to the contragredient rep $\tilde{\mathcal{D}}^{-1}$.

In atomic or nuclear physics, $[\nu] = [1]$ corresponds to a single particle state, while $[1^{n-1}]$ corresponds to a single hole state, and $[1^n]$ is the closed shell state. The relation between $[\nu_1 \nu_2 \ldots \nu_n]$ and its contragredient rep $[\nu'_1 \nu'_2 \ldots \nu'_n]$ is that of particle–hole conjugation.

If a partition $[\nu] = [\nu_1, \nu_2 \ldots]$ satisfies

$$\nu_p + \nu_{n-p+1} = \nu_1 \ , \quad p = 1, 2, \ldots, n \ , \tag{7-86}$$

then $[\nu'] = [\nu]$, that is, the irrep $[\nu]$ and its contragredient rep are equivalent. Thus for the group SU_5 we have, for example, $[\nu] = [\nu'] = [4321]$, $[\nu] = [\nu'] = [4222]$, and $[\nu] = [\nu'] = [21^3]$. These examples are illustrated in Fig. 7.6-2.

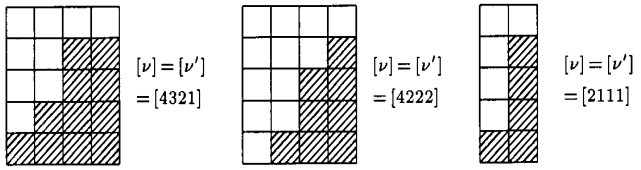


Fig. 7.6-2. Some reps of SU_5 with equivalent contragredient reps

It is easily seen that the adjoint rep $[\nu_0] = [21^{n-1}]$ of SU_n obeys the condition (7-86). Therefore $D^{[\nu_0]} = D^{[\nu'_0]} = (\tilde{D}^{[\nu_0]})^{-1} = (D^{[\nu_0]})^*$, that is, the adjoint rep is equivalent to a real rep. The adjoint rep [2] of SU_2 (corresponding to $J = 1$), for instance, is equivalent to the real rep $\mathcal{D}(\alpha\beta\gamma)$ of (5-34).

It follows from (7-82) that for the SU_3 group, the contragredient rep of the irrep $(\lambda\mu)$ is $(\mu\lambda)$.

7.7. The CG Coefficients of SU_n Group

Suppose $[\nu_1]$ and $[\nu_2]$ are two irreps of SU_n. Their CG series is denoted by

$$[\nu_1] \times [\nu_2] = \sum_{\nu} \{\nu_1 \nu_2 \nu\} [\nu] \,. \tag{7-87}$$

The two irreducible basis $\left| \begin{matrix} [\nu_1] \\ w_1 \end{matrix} \right\rangle$ and $\left| \begin{matrix} [\nu_2] \\ w_2 \end{matrix} \right\rangle$ can be coupled together to give another irreducible basis $\left| \begin{matrix} [\nu]_\tau \\ w \end{matrix} \right\rangle$ of SU_n by means of the CG coefficients

$$\left| \begin{matrix} [\nu]_\tau \\ w \end{matrix} \right\rangle = \sum_{w_1 w_2} C^{[\nu]\tau, w}_{\nu_1 w_1, \nu_2 w_2} \left| \begin{matrix} [\nu_1] \\ w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ w_2 \end{matrix} \right\rangle ,$$
$$\tau = 1, 2, \ldots, \{\nu_1 \nu_2 \nu\} \,, \tag{7-88a}$$

where w_1, w_2 and w are component indices.

The CG coefficients of SU_n satisfy the unitarity condition

$$\sum_{w_1 w_2} C^{[\nu]\tau, w}_{\nu_1 w_1, \nu_2 w_2} C^{[\nu']\tau', w'}_{\nu_1 w_1, \nu_2 w_2} = \delta_{\nu\nu'} \delta_{\tau\tau'} \delta_{ww'} \,, \tag{7-89a}$$

$$\sum_{\nu \tau W} C^{[\nu]\tau, W}_{\nu_1 w_1, \nu_2 w_2} C^{[\nu]\tau, W}_{\nu_1 w_1', \nu_2 w_2'} = \delta_{w_1 w_1'} \delta_{w_2 w_2'} \,. \tag{7-89b}$$

The inverse of (7-88a) is

$$\left| \begin{matrix} [\nu_1] \\ w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ w_2 \end{matrix} \right\rangle = \sum_{\nu \tau w} C^{[\nu]\tau, w}_{\nu_1 w_1, \nu_2 w_2} \left| \begin{matrix} [\nu]_\tau \\ w \end{matrix} \right\rangle \,. \tag{7-88b}$$

7.7.1. The CG coefficients of U_n and the IDC of the permutation group

The CG coefficients of a group depend on the particular basis we use. In this section we restrict ourselves to the CG coefficients for the Gel'fand basis of SU_n. The CG coefficients of SU_n for other kinds of basis will be discussed in Sec. 7.13.

The problem of the CG coefficients of SU_2 was solved a long time ago by Wigner (see Rose 1957). Those are the well known coupling coefficients of angular momentum. The CG coefficients of SU_n with $n \geq 3$ are usually calculated by Racah's infinitesimal operator method (Racah 1951). Systematic tables are available only for the CG coefficients of SU_3 (de Swart 1963) and SU_4 (Rabl 1975, Haacke 1976). Biedenharn (1967) discussed a canonical definition of the CG coefficients for U_n.

As n gets larger, the calculation of the SU_n CG coefficients by Racah's method becomes increasingly unwieldy. We are going to introduce a new method for evaluating the CG coefficients of the SU_n Gel'fand basis from the IDC of the permutation group. The distinguishing advantage of the new method is that the calculation is rank independent. We first discuss the U_n CG coefficients.

1. *The case without identical single particle states in the Weyl tableaux.* The outer-product in Sec. 4.14 refers to the coordinate-permutation group S_f. We now generalize it to the state-permutation group $\mathcal{S}_f$. First we assume that all the f single particle states are distinct. In such a case, the groups $\mathcal{S}_f$ and S_f are on the same footing. Interpreting the indices of the particle coordinates as indices of the single particle states, the standard bases $|Y_m^{(\nu)\tau}(\omega^0)\rangle$ and $|Y_{m_i}^{(\nu_i)}(\omega_i)\rangle$

of the permutation groups become the Gel'fand bases $\left|\begin{matrix}[\nu]\tau \\ w\end{matrix}\right\rangle$ and $\left|\begin{matrix}[\nu_i] \\ w_i\end{matrix}\right\rangle$; therefore (4-141) can be rewritten as

$$\left|\begin{matrix}[\nu]_\tau \\ w\end{matrix}\right\rangle = \sum_{m_1\omega_1 m_2\omega_2} C^{[\nu]\tau,m}_{\nu_1 m_1\omega_1,\nu_2 m_2\omega_2} \left|\begin{matrix}[\nu_1] \\ w_1\end{matrix}\right\rangle \left|\begin{matrix}[\nu_2] \\ w_2\end{matrix}\right\rangle . \tag{7-90}$$

Comparing (7-88a) with (7-90), we have

$$C^{[\nu]\tau,m}_{\nu_1 m_1\omega_1,\nu_2 m_2\omega_2} = C^{[\nu]\tau,w}_{\nu_1 w_1,\nu_2 w_2} , \tag{7-91}$$

that is, the IDC of S_f are just the CG coefficients of the U_f Gel'fand bases without identical single particle states in their Weyl tableaux. Thus the IDC tables are also the tables of the CG coefficients of U_f. By means of index substitutions, we can further obtain the CG coefficients of U_n with arbitrary $n \geq f$. Suppose that we have n single particle states $\alpha, \beta, \gamma, \ldots, \delta$ with the convention that the state are ordered as $\alpha < \beta < \gamma < \ldots < \delta$. A series of tables for the CG coefficients of U_n can be obtained by making the following index substitution for the Young tableaux $Y^{(\nu)}_m, Y^{(\nu_1)}_{m_1}$ and $Y^{(\nu_2)}_{m_2}$ in the IDC table of the permutation group $S_f (f \leq n)$:

$$1 \to i_1 , \quad 2 \to i_2 , \ldots, f \to i_f ,$$

where $i_1, i_2, \ldots, i_f$ are the f single particle states chosen arbitrarily from among the n single particle states $\alpha, \beta, \gamma, \ldots, \delta$ under the restriction that $i_1 < i_2 < i_3 < \ldots < i_f$. As an example, take $n = 6$. We have six single particle states $\alpha, \beta, \gamma, \delta, \varepsilon, \varphi$. $\binom{6}{4} = 15$ tables of the U_6 CG coefficients are obtained from the following index substitution for each IDC table in Table 4.17:

$$\begin{aligned}(1234) \to\ & (\alpha\beta\gamma\delta) , \quad (\alpha\beta\gamma\varepsilon) , \quad (\alpha\beta\gamma\varphi) , \quad (\alpha\beta\delta\varepsilon) , \quad (\alpha\beta\delta\varphi) , \\ & (\alpha\beta\varepsilon\varphi) , \quad (\alpha\gamma\delta\varepsilon) , \quad (\alpha\gamma\delta\varphi) , \quad (\alpha\gamma\varepsilon\varphi) , \quad (\alpha\delta\varepsilon\varphi) , \\ & (\beta\gamma\delta\varepsilon) , \quad (\beta\gamma\delta\varphi) , \quad (\beta\gamma\varepsilon\varphi) , \quad (\beta\delta\varepsilon\varphi) , \quad (\gamma\delta\varepsilon\varphi) .\end{aligned}$$

Thus it can be seen that simply by index substitutions, each IDC table gives rise to an infinite number of CG coefficient tables of unitary groups.

2. *The case with identical single particle states in the Weyl tableaux.* If we let the coordinate indices in (4-142a) go over to the state indices according to the following:

$$\begin{aligned}(12\ldots f) \to (i_1 i_2 \ldots i_f) , \quad & i_1 \leq i_2 \leq \ldots \leq i_f , \\ (\omega^0) \to (\overline{\omega}^0) = (i_1 i_2 \ldots i_f) , \quad & (\omega_1) = (a_1 \ldots a_{f_1}) \to (\overline{\omega}_1) = (i_{a_1} \ldots i_{a_{f_1}}) , \\ & (\omega_2) = (a_{f_1+1} \ldots a_f) \to (\overline{\omega}_2) = (i_{a_{f_1+1}} \ldots i_{a_f}) ,\end{aligned} \tag{7-92}$$

then the normal order sequences (ω^0) and (ω_i) go over to the normal order states $(\overline{\omega}^0)$ and $(\overline{\omega}_i)$, respectively.

In the following we want to show that (4-141) still holds when there are identical single particle states in the normal order state $(\overline{\omega}^0) = (i_1 i_2 \ldots i_f)$.

Taking the Hermitian conjugation of (4-176b) and using (3-242d),

$$\mathcal{P}^{[\nu]m}_{\tau[\nu_1]m'_1[\nu_2]m'_2} = \sum_{m_1 m_2 \omega} C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2,\omega} P^{[\nu_1]m_1}_{m'_1} P^{[\nu_2]m_2}_{m'_2} (Q_\omega)^{-1} . \tag{7-93a}$$

Applying it to the normal order state $(\overline{\omega}^0) = (i_1 i_2 \ldots i_f)$ we have

$$\mathcal{P}^{[\nu]m}_{\tau[\nu_1]m'_1[\nu_2]m'_2} |\overline{\omega}^0\rangle = \sum_{m_1\omega_1 m_2\omega_2} C^{[\nu]\tau,m}_{\nu_1 m_1,\nu_2 m_2,\omega} P^{[\nu_1]m_1}_{m'_1} |\bar{\omega}_1\rangle P^{[\nu_2]m_2}_{m'_2} |\bar{\omega}_1\rangle . \tag{7-93b}$$

where we used (3-110) and

$$(Q_\omega)^{-1}|\overline{\omega}^0\rangle = Q_\omega|\overline{\omega}^0\rangle = |\overline{\omega}\rangle.$$

Ignoring the lower indices in (7-93b) (since we are interested only in the irreducible basis in the state space), Eq. (7-93b) is identical to (4-141) but extended to the state space with repeated single particle states, namely

$$|Y^{[\nu]\tau}_m(\bar{\omega}^0)\rangle = \sum_{m_1\omega_1 m_2\omega_2} C^{[\nu]\tau,m}_{\nu_1 m_1\omega_1,\nu_2 m_2\omega_2}|Y^{[\nu_1]}_{m_1}(\bar{\omega}_1)\rangle|Y^{[\nu_2]}_{m_2}(\bar{\omega}_2)\rangle\ . \tag{7-93c}$$

When there are identical single particle states, $|Y^{[\nu]\tau}_m(\overline{\omega}^0)\rangle$ and $|Y^{[\nu_i]}_{m_i}(\overline{\omega}_i)\rangle$ are the unnormalized Gel'fand bases of U_n. From (4-81a) and (4-86) we have

$$|Y^{[\nu]}_m(\overline{\omega}^0)\rangle = R^{[\nu]m}(\overline{\omega}^0)\left|\begin{matrix}[\nu]\\ w\end{matrix}\right\rangle\ , \tag{7-94a}$$

$$|Y^{[\nu_i]}_{m_i}(\overline{\omega}_i)\rangle = R^{[\nu_i]m_i}(\overline{\omega}_i)\left|\begin{matrix}[\nu_i]\\ w_i\end{matrix}\right\rangle\ . \tag{7-94b}$$

It must be stressed that in (7-94a) there may be several m which give rise to the same Weyl tableau w, and in (7-94b) there may be several m_i which give rise to the same Weyl tableaux w_i. A Gel'fand basis vector vanishes whenever there are identical single particle states appearing in the same column of the Weyl tableau.

Substituting (7-94) into (7-93c) and making use of (7-88), we get the general relation between the CG coefficients of U_n and the IDC of the permutation groups,

$$C^{[\nu]\tau,w}_{\nu_1 w_1,\nu_2 w_2} = \frac{1}{R^{[\nu]m}(\overline{\omega}^0)}\sum_{\substack{m_1 m_2\\ \omega_1\omega_2}}{}' R^{[\nu_1]m_1}(\overline{\omega}_1)R^{[\nu_2]m_2}(\overline{\omega}_2)C^{[\nu]\tau,m}_{\nu_1 m_1\omega_1,\nu_2 m_2\omega_2}\ , \tag{7-95}$$

where the prime in the summation symbol indicates that the sum runs over only those m_i which will give rise to the same Weyl tableaux w_i, and the relations between $(\overline{\omega}^0), (\overline{\omega}_i)$ and $(\omega^0), (\omega_i)$ are specified by (7-92).

When there are no identical single particle states in $(\overline{\omega}^0)$ the correspondence between $m_i\overline{\omega}_i$ and w_i is one–to–one. Only one term on the right–hand side of (7-95) then survives, and (7-95) therefore reduces to the special case (7-91).

An important conclusion obtained from the above discussion is that the *value of the U_n CG coefficients do not depend explicitly on n.* Once the IDC are known, with the help of some universal (and positive) normalization constants $R^{[\nu]m}(\omega)$ which can be evaluated easily by the method of Chen & Chen (1983), the CG coefficients of any U_n group can be found from (7-95) in one stroke, without the need to calculate them for one n at a time.

Note that the left–hand side of (7-95) is independent of the quantum number m. Therefore in practical calculations, m can take any possible value as long as (7-94a) is satisfied.

The relation (7-95) between the CG coefficients of U_n and the IDC of the permutation group also tells us about the CG series of SU_n. Namely, the irreps $[\nu]$ contained in the product of two irreps $[\nu_1]$ and $[\nu_2]$ of SU_n are determined by the Littlewood rule under the restriction that one has to disregard the Young diagrams $[\nu]$ of more than n rows and delete the columns of length n in any Young diagram $[\nu]$.

For example, from (4-136) we find the CG series for the groups U_3 and SU_3 to be

$$\begin{aligned} U_3 &: [21]\times[21] = [42] + [411] + [33] + 2[321] + [222]\ ,\\ SU_3 &: [21]\times[21] = [42] + [3] + [33] + 2[21] + [0]\ . \end{aligned} \tag{7-96}$$

As a dimension check[2], $8 \times 8 = 27 + 10 + 1 + 2 \times 8 + 1$. Similarly, for SU_4 we have

$$SU_4 : [21] \times [21] = [42] + [411] + [33] + 2[321] + [222] + [2] + [11] . \tag{7-97}$$

We note again that $20 \times 20 = 126 + 70 + 50 + 2 \times 64 + 10 + 10 + 6$.

7.7.2. The procedure for evaluating the SU_n CG coefficients

1. Pick out the typical normal order states. Suppose the single particle states $\alpha, \beta, \gamma, \ldots, \varepsilon$ span the fundamental rep of U_n. There are altogether $\binom{n+f-1}{f}$ normal order states $|\overline{\omega}^0\rangle = |i_1, i_2 \ldots i_f\rangle, i = \alpha, \beta, \gamma, \ldots, \varepsilon$. We only need to calculate the CG coefficients for some typical normal order states. Thus for $f = 4$ and $n = 4$, there are 35 normal order states, but only the following eight states are typical ones:

$$|\alpha\beta\gamma\delta\rangle , \quad |\alpha\alpha\beta\gamma\rangle , \quad |\alpha\beta\beta\gamma\rangle , \quad |\alpha\beta\gamma\gamma\rangle , \quad |\alpha\alpha\beta\beta\rangle , \quad |\alpha\alpha\alpha\beta\rangle , \quad |\alpha\beta\beta\beta\rangle , \quad |\alpha\alpha\alpha\alpha\rangle .$$

The CG coefficients for the first case are simply the IDC; the CG coefficients for the last case are trivial, while the CG coefficients for cases 5, 6 and 7, are just the SU_2 CG coefficients which have been tabulated (Rotenberg 1959). Therefore only the CG coefficients for the three normal order states $|\overline{\omega}^0\rangle = |\alpha\alpha\beta\gamma\rangle, |\alpha\beta\beta\gamma\rangle$ and $|\alpha\beta\gamma\gamma\rangle$ need to be calculated.

Once the CG coefficients for the above typical cases are known, all the CG coefficients of any U_n group for four-particle system are obtained merely through index substitutions. For example, the CG coefficients of U_5 can be obtained from those of U_4 by setting

$$\begin{aligned} |\overline{\omega}^0\rangle = |\alpha\beta\gamma\delta\rangle = |1234\rangle , \quad |1235\rangle , \quad |1245\rangle , \quad |1345\rangle , \quad |2345\rangle , \\ |\overline{\omega}^0\rangle = |\alpha\alpha\beta\gamma\rangle = |1123\rangle , \quad |1124\rangle , \quad |2234\rangle , \quad \ldots , \quad |3345\rangle . \end{aligned} \tag{7-98}$$

2. Change the headings in the IDC tables. By making the following substitutions $1 \to i_1, 2 \to i_2, \ldots, f \to i_f$, the Young tableaux in the headings of the IDC tables become the Weyl tableaux:

$$Y_m^{[\nu]}(\overline{\omega}^0) \to w , \quad Y_{m_i}^{[\nu_1]}(\overline{\omega}_i) \to w_i . \tag{7-99}$$

3. Divide the entries in the row $[\nu]m$ of the IDC table with $R^{[\nu]m}(\overline{\omega}^0)$, and multiply the entries in the column labelled $m_1\omega_1 m_2\omega_2$ with $R^{[\nu_1]m_1}(\overline{\omega}_1)R^{[\nu_2]m_2}(\overline{\omega}_2)$. The norms $R^{[\nu]m}(\omega)$ for $S_f, f \leq 5$, are listed in Table 4.8.

4. Finally the CG coefficients are obtained by summing up the entries under the same heading (w_1, w_2).

To illustrate, Table 7.7-1a gives the IDC of S_3 (the table is taken from Table 4.17-2). By letting $(\overline{\omega}^0) = (\alpha\alpha\beta)$, the Young tableaux in Table 7.7-1a go over to the Weyl tableaux in Table 7.7-1b, where in the third row there are two $\alpha's$ in the same column so that $\left|\begin{smallmatrix}\alpha\beta\\ \alpha\end{smallmatrix}\right\rangle = 0$.

Dividing the first and second row in Table 7.7-1a with $R^{[3]}(\alpha\alpha\beta) = R^{[21]}(\alpha\alpha\beta) = \sqrt{2}$, and multiplying the first, second and third columns by $R^{[2]}(\alpha\alpha) = \sqrt{2}, R^{[2]}(\alpha\beta) = 1$ and $R^{[2]}(\alpha\beta) = 1$, respectively, we get Table 7.7-1b. The CG coefficients of U_n result from adding the second and third columns in Table 7.7-1b and are shown in Table 7.7-1c.

As can be seen, the coefficients in Table 7.7-1c are precisely the SU_2 CG coefficients (including the phase).

Analogously, from the $[21] \times [1]$ IDC in Table 4.17-3d, we find the CG coefficients of U_n given in Table 7.7-2.

7.7.3 Phase conventions

There are two phase choices to consider.

[2]The dimension tables are given in Table A.1 in the Appendix.

Table 7.7-1a. $[2]\times[1]$ IDC of S_3.

	$\boxed{1}\boxed{2}\boxed{3}$	$\boxed{1}\boxed{3}\boxed{2}$	$\boxed{2}\boxed{3}\boxed{1}$
$\boxed{1}\boxed{2}\boxed{3}$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{3}}$
$\begin{array}{\|c\|c\|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}$	$\sqrt{\frac{2}{3}}$	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$
$\begin{array}{\|c\|c\|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}$	0	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$

Table 7.7-1b. The intermediate step.

	$\boxed{\alpha}\boxed{\alpha}\boxed{\beta}$	$\boxed{\alpha}\boxed{\beta}\boxed{\alpha}$	$\boxed{\alpha}\boxed{\beta}\boxed{\alpha}$
$\boxed{\alpha}\boxed{\alpha}\boxed{\beta}$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$
$\begin{array}{\|c\|c\|}\hline \alpha&\alpha\\\hline \beta\\\cline{1-1}\end{array}$	$\sqrt{\frac{2}{3}}$	$-\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$
$\begin{array}{\|c\|c\|}\hline \alpha&\beta\\\hline \alpha\\\cline{1-1}\end{array}$			

Table 7.7-1c. The CG coefficients of U_n.

	$\boxed{\alpha}\boxed{\alpha}\boxed{\beta}$	$\boxed{\alpha}\boxed{\beta}\boxed{\alpha}$
$\boxed{\alpha}\boxed{\alpha}\boxed{\beta}$	$\frac{1}{\sqrt{3}}$	$\sqrt{\frac{2}{3}}$
$\begin{array}{\|c\|c\|}\hline \alpha&\alpha\\\hline \beta\\\cline{1-1}\end{array}$	$\sqrt{\frac{2}{3}}$	$-\frac{1}{\sqrt{3}}$

1. The relative phases of the IDC of S_f and CG coefficients of U_n. The Young–Yamanouchi phase convention for the IDC ensures that the CG coefficients of U_n calculated from (7-95) fulfill the Gel'fand–Biedenharn phase convention (see Sec. 7.5).

2. The overall phase. By (7-95), the overall phases of the CG coefficients of SU_n and the IDC of the permutation group are closely related. The overall phase convention (4-146) for the IDC ensures that the CG coefficients of SU_n derived from (7-95) satisfy the Baird–Biedenharn (1965) phase convention which demands that the CG coefficient associated with the highest weight (hw) be positive, that is

$$C^{[\nu]\tau,hw}_{\nu_1 hw_1,\nu_2 w_2} > 0\ . \tag{7-100}$$

The highest weight state $|[\nu]hw\rangle$ is defined as the state formed by filling the Young diagram $[\nu]$ in the following way: The boxes in the first row are all filled with 1 (or α), and the boxes in the second row with 2 (or β), and so on.

The convention (7-100) is a generalization of the Condon–Shortley phase convention that demands $C^{JJ}_{j_1 j_1, j_2 J-j_1} > 0$, for the CG coefficients of SU_2. The phase convention (7-100) ensures that *our U_n CG coefficients are also the SU_n CG coefficients.*

From (7-95) and (4-153a) it is known that the CG coefficients of SU_n has the symmetry

$$C^{[\nu]\tau,w}_{\nu_1 w_1,\nu_2 w_2} = \varepsilon_1 C^{[\nu]\tau,w}_{\nu_2 w_2,\nu_1 w_1}\ . \tag{7-101}$$

The phase factor ε_1 is given by (4-153b) and tabulated in Table A.2 of the Appendix.

The CG coefficients for the SU_n Gel'fand basis are tabulated in a rank independent way in Chen, Wang, Lü and Wu (1987) for partitions of integers up to six.

Ex. 7.5. Construct the CG series of SU_3 for $[31]\times[22]$.

Ex. 7.6. Construct the four-quark state $\left|\begin{matrix}uus\\ d\end{matrix}\right\rangle$ in terms of P, $\Sigma^+,\Sigma^0,\Lambda^0$ and a single quark state.

Ex. 7.7. Change the component indices and the Weyl tableaux in Table 7.7-2 to the quantum number II_zY.

Table 7.7-2. $[21]\times[1]$ CG coefficients of U_n.

$[21]\otimes[1]$

	$\begin{matrix}\alpha\alpha\\ \beta\end{matrix},\gamma$	$\begin{matrix}\alpha\alpha\\ \gamma\end{matrix},\beta$	$\begin{matrix}\alpha\beta\\ \gamma\end{matrix},\alpha$	$\begin{matrix}\alpha\gamma\\ \beta\end{matrix},\alpha$
$\begin{matrix}\alpha\alpha\beta\\ \gamma\end{matrix}$	0	$\frac{1}{\sqrt{3}}$	$\sqrt{\frac{2}{3}}$	0
$\begin{matrix}\alpha\alpha\gamma\\ \beta\end{matrix}$	$\sqrt{\frac{3}{8}}$	$\frac{1}{\sqrt{24}}$	$-\frac{1}{\sqrt{48}}$	$\frac{3}{4}$
$\begin{matrix}\alpha\alpha\\ \beta\\ \gamma\end{matrix}$	$\sqrt{\frac{3}{8}}$	$-\sqrt{\frac{3}{8}}$	$\frac{\sqrt{3}}{4}$	$-\frac{1}{4}$
$\begin{matrix}\alpha\alpha\\ \beta\gamma\end{matrix}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{\sqrt{8}}$	$-\sqrt{\frac{3}{8}}$

$[21]\otimes[1]$

	$\begin{matrix}\alpha\beta\\ \beta\end{matrix},\gamma$	$\begin{matrix}\alpha\beta\\ \gamma\end{matrix},\beta$	$\begin{matrix}\beta\beta\\ \gamma\end{matrix},\alpha$	$\begin{matrix}\alpha\gamma\\ \beta\end{matrix},\beta$
$\begin{matrix}\alpha\beta\beta\\ \gamma\end{matrix}$	0	$\sqrt{\frac{2}{3}}$	$\sqrt{\frac{1}{3}}$	0
$\begin{matrix}\alpha\beta\gamma\\ \beta\end{matrix}$	$\sqrt{\frac{3}{8}}$	$\frac{1}{\sqrt{48}}$	$-\frac{1}{\sqrt{24}}$	$\frac{3}{4}$
$\begin{matrix}\alpha\beta\\ \beta\\ \gamma\end{matrix}$	$\sqrt{\frac{3}{8}}$	$-\frac{\sqrt{3}}{4}$	$\sqrt{\frac{3}{8}}$	$-\frac{1}{4}$
$\begin{matrix}\alpha\beta\\ \beta\gamma\end{matrix}$	$\frac{1}{2}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{2}$	$-\sqrt{\frac{3}{8}}$

$[21]\otimes[1]$

	$\begin{matrix}\alpha\beta\\ \gamma\end{matrix},\gamma$	$\begin{matrix}\alpha\gamma\\ \beta\end{matrix},\gamma$	$\begin{matrix}\alpha\gamma\\ \gamma\end{matrix},\beta$	$\begin{matrix}\beta\gamma\\ \gamma\end{matrix},\alpha$
$\begin{matrix}\alpha\beta\gamma\\ \gamma\end{matrix}$	$\sqrt{\frac{1}{2}}$	0	$\frac{1}{2}$	$\frac{1}{2}$
$\begin{matrix}\alpha\gamma\gamma\\ \beta\end{matrix}$	0	$\frac{\sqrt{3}}{2}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$
$\begin{matrix}\alpha\gamma\\ \beta\\ \gamma\end{matrix}$	0	$\frac{1}{2}$	$-\sqrt{\frac{3}{8}}$	$-\sqrt{\frac{3}{8}}$
$\begin{matrix}\alpha\beta\\ \gamma\gamma\end{matrix}$	$\sqrt{\frac{1}{2}}$	0	$-\frac{1}{2}$	$-\frac{1}{2}$

7.8 The CG Coefficients of SU_n and the $S_f \supset S_{f_1}\otimes S_{f_2}$ Irreducible Basis

Let

$$\left|\begin{matrix}[\nu_i]\\ m_i\omega_i^0,\ w_i\end{matrix}\right\rangle = |Y_{m_i}^{[\nu_i]}(\omega_i^0), w_i)\ ,$$
$$(\omega_1^0) = (1,2,\ldots,f_1)\ ,\quad (\omega_2^0) = (f_1+1,\ldots,f_1+f_2)\ , \tag{7-102a}$$

be the irreducible basis $[\nu_i]m_i$ of the permutation group $S_{f_i} = S_{f_i}(\omega_i^0)$ and the irreducible basis $[\nu_i]w_i$ of the unitary group SU_n.

Theorem 7.3: The CG coefficients of SU_n are the indirect coupling coefficients for $S_f \supset S_{f_1}\otimes S_{f_2}$ irreducible basis ($f = f_1 + f_2$), namely,

$$\left|\begin{matrix}[\nu]\\ \theta[\nu_1]m_1[\nu_2]m_2,\ w\end{matrix}\right\rangle = \sum_{w_1 w_2} C_{\nu_1 w_1,\nu_2 w_2}^{[\nu]\theta,w}\left|\begin{matrix}[\nu_1]\\ m_1\omega_1^0,\ w_1\end{matrix}\right\rangle\left|\begin{matrix}[\nu_2]\\ m_2\omega_2^0,\ w_2\end{matrix}\right\rangle . \tag{7-102b}$$

Proof: According to the definition of the CG coefficients of SU_n, the right-hand side of (7-102b) belongs to the irrep $[\nu]$ of SU_n, and in view of Theorem 7.1 it must also belong to the irrep $[\nu]$ of S_f. The quantum numbers $[\nu_i]m_i$ are also fixed in (7-102b), and therefore (7-102b) remains the irreducible basis $[\nu_1]m_1$ of S_{f_1} and $[\nu_2]m_2$ of S_{f_2}. In other words, (7-102b) is the irreducible basis $|\nu w\rangle$ of SU_n and the $S_f \supset S_{f_1}\otimes S_{f_2}$ irreducible basis.

Using (4-168b), we can transfer the non-standard basis of S_f to the standard basis of S_f:

$$\left|\begin{matrix}[\nu]\\ m,\ w\end{matrix}\right\rangle = \sum_{\nu_2 m_2 \theta w_1 w_2}\left\langle\begin{matrix}[\nu]\\ m\end{matrix}\middle|[\nu],\begin{matrix}\theta[\nu_1][\nu_2]\\ m_1\quad m_2\end{matrix}\right\rangle C_{\nu_1 w_1,\nu_2 w_2}^{[\nu]\theta,w}\left|\begin{matrix}[\nu_1]\\ m_1\omega_1^0, w_1\end{matrix}\right\rangle\left|\begin{matrix}[\nu_2]\\ m_2\omega_2^0, w_2\end{matrix}\right\rangle . \tag{7-102c}$$

7.9. The $SU_{mn} \supset SU_m \times SU_n$ Irreducible Basis

7.9.1. The CG coefficients of S_f and the $SU_{mn} \supset SU_m \times SU_n$ irreducible basis

A particle usually has several kinds of degrees of freedom. For example, a nucleon has the degrees of freedom in the orbital space V^x, spin space V^σ and isospin space V^τ. A nucleon with orbital angular momentum l has $n = 4(2l+1)$ states altogether.

In many cases, the permutation symmetry $[\nu]$ in orbital space, the total spin S and the total isospin T are good, or approximately good quantum numbers (for example, when the nuclear force is the Serber force, $V_{ij} = v(r_{ij})(W + M^x p_{ij})$ where W and M are constants, and ${}^x p_{ij}$ is the permutation operator in orbital space). Therefore it is most convenient to use basis functions with definite space symmetry $[\nu]$, definite spin S and isospin T, namely, we need $SU_{4(2l+1)} \supset SU_{2l+1} \times SU_2 \times SU_2$ irreducible basis, rather than the Gel'fand basis. In this section, we will give a general method for constructing such a type of basis. We begin with two types of degrees of freedom, that is we shall consider the $SU_{mn} \supset SU_m \times SU_n$ irreducible basis. For example the $SU_4 \supset SU_2 \times SU_2$ in nuclear physics and the $SU_6 \supset SU_3^{(f)} \times SU_2^{(\sigma)}$ or $SU_8 \supset SU_4^{(f)} \times SU_2^{(\sigma)}$ in particle physics where f indicates flavor space.

Consider the following three kinds of f–particle product states:

$$x\text{–space:}\quad \varphi = \varphi_{i_1}(x_1)\dots\varphi_{i_f}(x_f)\ ,\quad i_1\dots i_f = 1,2,\dots m\ , \tag{7-103a}$$

$$\xi\text{–space:}\quad x = \chi_{\alpha_1}(\xi_1)\dots\chi_{\alpha_f}(\xi_f)\ ,\quad \alpha_1\dots\alpha_f = 1,2,\dots n\ , \tag{7-103b}$$

$$q\text{–space:}\quad \psi = \psi_{s_1}(q_1)\dots\psi_{s_f}(q_f)\ ,\quad s = (i,\alpha) = (1,1),\dots(1,n),(2,1),\dots(m,n)\ , \tag{7-103c}$$

where

$$q = (x,\xi)\ ,\quad \psi_s(q) = \varphi_i(x)\chi_\alpha(\xi)\ ,$$

$$\begin{pmatrix} \varphi_1\dots\varphi_m \\ \chi_1\dots\chi_n \\ \psi_{1,1}\dots\psi_{m,n} \end{pmatrix} \text{carry the fundamental reps of} \begin{pmatrix} SU_m \\ SU_n \\ SU_{mn} \end{pmatrix}\ .$$

To avoid repetitive statements, we use a straightforward shorthand notation. For example, in the SU_6 model of elementary particles, x represents flavor space with φ_1, φ_2 and φ_3 representing the quark states u, d and s, while ξ represents spin space, $\chi_1(\chi_2)$ being the spin-up (spin-down) state $\chi_\alpha(\chi_\beta)$, and in q space, $s = (u\alpha),(u\beta),(d\alpha),(d\beta),(s\alpha),(s\beta)$ carry the fundamental rep of SU_6.

The group elements of SU_m, SU_n and SU_{mn} are the following matrices, respectively,

$$U_{ij}(a^1\dots a^{r_m})\ ,\quad U_{\alpha\beta}(b^1\dots b^{r_n})\ ,\quad U_{i\alpha,j\beta}(c^1\dots c^r)\ ,$$
$$r_m = m^2-1\ ,\quad r_n = n^2-1\ ,\quad r = (mn)^2-1\ , \tag{7-104a}$$

where r_m, r_n and r are the orders of the three groups. $U_{ij}, U_{\alpha\beta}$ and $U_{i\alpha,j\beta}$ are $m\times m, n\times n$ and $mn\times mn$ matrices, respectively. Notice that the group $SU_m \times SU_n$ consists of the unitary matrices

$$U_{i\alpha,j\beta}(a^1\dots a^{r_m}, b^1\dots b^{r_n}) = U_{ij}(a^1\dots a^{r_m})U_{\alpha\beta}(b^1\dots b^{r_n}) \tag{7-104b}$$

with order $r_m + r_n = m^2 + n^2 - 2$. Obviously, $SU_m \times SU_n$ is a subgroup of SU_{mn}.

The f–particle product states $\begin{pmatrix} \varphi \\ \chi \\ \psi \end{pmatrix}$ carry a reducible rep of $\begin{pmatrix} S_f(\chi) \\ S_f(\xi) \\ S_f(q) \end{pmatrix}$ as well as one of $\begin{pmatrix} SU_m \\ SU_n \\ SU_{mn} \end{pmatrix}$. Assume that

$$\varphi^{[\nu_1]}_{m_1}(x, w_1) = \left| \begin{matrix} [\nu_1] \\ m_1, w_1 \end{matrix} \right\rangle \tag{7-105a}$$

is the standard basis $[\nu_1]m_1$ of $S_f(x)$ and the irreducible basis $[\nu_1]w_1$ of SU_m, and let

$$\chi^{[\nu_2]}_{m_2}(\xi, w_2) = \left| \begin{matrix} [\nu_2] \\ m_2\ , w_2 \end{matrix} \right\rangle \tag{7-105b}$$

be the standard basis $[\nu_2]m_2$ of $S_f(\xi)$ and the irreducible basis $[\nu_2]w_2$ of SU_n, where w_1 and w_2 are component indices of the irreps of SU_m and SU_n, respectively. For clarity, we assume that w_1 and w_2 are labels for the Gel'fand bases of SU_m and SU_n, although the following discussion is independent of classification of the irreducible bases of SU_m and SU_n. Therefore w_1 and w_2 may represent two Weyl tableaux filled with the state indices $i_1, i_2, \ldots, i_f$ and $\alpha_1, \alpha_2 \ldots, \alpha_f$, respectively. To illustrate, we have

$$\left| \begin{matrix} [\nu_1] \\ m_1 = 1, w_1 \end{matrix} \right\rangle = \left| \begin{array}{|c|c|}\hline u & d \\ \hline s \\ \cline{1-1} \end{array} \right\rangle_1 = \left| \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 \\ \cline{1-1} \end{array} \quad \begin{array}{|c|c|}\hline u & d \\ \hline s \\ \cline{1-1} \end{array} \right\rangle ,$$

$$\left| \begin{matrix} [\nu_2] \\ m_2 = 2, w_2 \end{matrix} \right\rangle = \left| \begin{array}{|c|c|}\hline \alpha & \alpha \\ \hline \beta \\ \cline{1-1} \end{array} \right\rangle_2 = \left| \begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 \\ \cline{1-1} \end{array} \quad \begin{array}{|c|c|}\hline \alpha & \alpha \\ \hline \beta \\ \cline{1-1} \end{array} \right\rangle ,$$

where the state $\left| \begin{matrix} [\nu_1] \\ m_1\ w_1 \end{matrix} \right\rangle$ and $\left| \begin{matrix} [\nu_2] \\ m_2\ w_2 \end{matrix} \right\rangle$ are linear combinations of the product states φ and χ, respectively.

In terms of the CG coefficients of permutation groups, (7-105) can be coupled into the Yamanouchi basis $[\nu]m$ of the group $S_f(q)$

$$\left| \begin{matrix} [\nu] \\ m, \beta[\nu_1]w_1[\nu_2]w_2 \end{matrix} \right\rangle = \left| \begin{matrix} [\nu]\beta[\nu_1][\nu_2] \\ m, \quad w_1 w_2 \end{matrix} \right\rangle = \sum_{m_1 m_2} C^{[\nu]\beta, m}_{\nu_1 m_1, \nu_2 m_2} \left| \begin{matrix} [\nu_1] \\ m_1 w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ m_2 w_2 \end{matrix} \right\rangle ,$$
$$\beta = 1, 2, \ldots, (\nu_1 \nu_2 \nu) . \tag{7-106a}$$

We now are going to prove that (7-106a) is the $[\nu]$ irreducible basis of SU_{mn}. According to the definition of the CG coefficients, (7-106a) is an eigenfunction of the CSCO-I $C(f)$ of $S_f(q)$. On account of (7-37), the invariants $I^{(mn)}_k$ of the group SU_{mn} for the basis (7-103c) are functions of the operator set $C(f)$ of $S_f(q)$:

$$I^{(mn)}_k = F^{(mn)}_k\big(C(f)\big) , \quad k = mn, mn-1, \ldots, 3, 2 . \tag{7-107}$$

Equation (7-107) remains true for the basis (7-106a), since (7-106a) are linear combinations of (7-103c). Therefore (7-106a) are also eigenfunctions of the CSCO $\{I^{(mn)}_k\}$ of SU_{mn}, which in turn means that (7-106a) are the bases of the irrep $[\nu]$ of SU_{mn}. Furthermore, since $\nu_1 w_1$ and $\nu_2 w_2$ in the right-hand side of (7-106a) are fixed, the left-hand side remains the irreducible basis of SU_m and SU_n. Therefore

$$\left| \begin{matrix} [\nu], \beta[\nu_1][\nu_2] \\ m, \quad w_1 w_2 \end{matrix} \right\rangle \quad \text{belongs to} \quad \begin{matrix} SU_{mn} \supset & SU_m & \times & SU_n, & S_f(q) \\ [\nu] & [\nu_1]w_1 & & [\nu_2]w_2 & [\nu]m \end{matrix} .$$

Thus we have

Theorem 7.4: The CG coefficients of the permutation group are the indirect coupling coefficients for the $SU_{mn} \supset SU_m \times SU_n$ irreducible basis.

Consequently, by utilizing the CG coefficients of the permutation group, we can easily construct the $SU_{mn} \supset SU_m \times SU_n$ irreducible bases for arbitrary m and n. Thus from (4-124) and (7-106a), we obtain the $SU_{mn} \supset SU_m \times SU_n$ basis for the totally anti-symmetric rep of $S_f(q)$ and SU_{mn},

$$\left| [1^f], \begin{matrix} [\nu][\tilde{\nu}] \\ w_1 w_2 \end{matrix} \right\rangle = \sum_m \frac{\Lambda^\nu}{\sqrt{h_\nu}} \left| \begin{matrix} [\nu] \\ m, w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\tilde{\nu}] \\ \tilde{m}, w_2 \end{matrix} \right\rangle . \tag{7-108}$$

Using the unitarity of the CG coefficients, (7-106a) can be inverted, giving

$$\left|\begin{matrix}[\nu_1]\\ m_1,w_1\end{matrix}\right\rangle\left|\begin{matrix}[\nu_2]\\ m_2,w_2\end{matrix}\right\rangle=\sum_{\nu\beta m} C^{[\nu]\beta,m}_{\nu_1 m_1,\nu_2 m_2}\left|\begin{matrix}[\nu],\beta[\nu_1][\nu_2]\\ m\quad w_1w_2\end{matrix}\right\rangle . \tag{7-106b}$$

Using the CG coefficients given in Table 4.13-1, the $SU_{mn}\supset SU_m\times SU_n$ (such as $SU_6\supset SU_3\times SU_2$ or $SU_8\supset SU_4\times SU_2$) baryon wave functions in the quark model can be expressed in terms of the following general formulas:

$$\begin{aligned}
&\left|[3],\begin{matrix}[21]&[21]\\ w_1&w_2\end{matrix}\right\rangle=\frac{1}{\sqrt{2}}\left[\left|\begin{matrix}[21]\\ w_1\end{matrix}\right\rangle_1\left|\begin{matrix}[21]\\ w_2\end{matrix}\right\rangle_1+\left|\begin{matrix}[21]\\ w_1\end{matrix}\right\rangle_2\left|\begin{matrix}[21]\\ w_2\end{matrix}\right\rangle_2\right],\\
&\left|[3],\begin{matrix}[3]&[3]\\ w_1&w_2\end{matrix}\right\rangle=\left|\begin{matrix}[3]\\ w_1\end{matrix}\right\rangle\left|\begin{matrix}[3]\\ w_2\end{matrix}\right\rangle,\\
&\left|[21],\begin{matrix}[3]&[21]\\ w_1&w_2\end{matrix}\right\rangle_m=\left|\begin{matrix}[3]\\ w_1\end{matrix}\right\rangle\left|\begin{matrix}[21]\\ w_2\end{matrix}\right\rangle_m,\\
&\left|[21],\begin{matrix}[21]&[3]\\ w_1&w_2\end{matrix}\right\rangle_m=\left|\begin{matrix}[21]\\ w_1\end{matrix}\right\rangle_m\left|\begin{matrix}[3]\\ w_2\end{matrix}\right\rangle,\\
&\left|[21],\begin{matrix}[21]&[21]\\ w_1&w_2\end{matrix}\right\rangle_1=\frac{1}{\sqrt{2}}\left[\left|\begin{matrix}[21]\\ w_1\end{matrix}\right\rangle_1\left|\begin{matrix}[21]\\ w_2\end{matrix}\right\rangle_1-\left|\begin{matrix}[21]\\ w_1\end{matrix}\right\rangle_2\left|\begin{matrix}[21]\\ w_2\end{matrix}\right\rangle_2\right],\\
&\left|[21],\begin{matrix}[21]&[21]\\ w_1&w_2\end{matrix}\right\rangle_2=-\frac{1}{\sqrt{2}}\left[\left|\begin{matrix}[21]\\ w_1\end{matrix}\right\rangle_1\left|\begin{matrix}[21]\\ w_2\end{matrix}\right\rangle_2+\left|\begin{matrix}[21]\\ w_1\end{matrix}\right\rangle_2\left|\begin{matrix}[21]\\ w_2\end{matrix}\right\rangle_1\right],\\
&\left|[21],\begin{matrix}[1^3]&[21]\\ w_1&w_2\end{matrix}\right\rangle_m=\Lambda^{[21]}_m\left|\begin{matrix}[1^3]\\ w_1\end{matrix}\right\rangle\left|\begin{matrix}[21]\\ w_2\end{matrix}\right\rangle_{\tilde{m}},\\
&\left|[1^3],\begin{matrix}[1^3]&[3]\\ w_1&w_2\end{matrix}\right\rangle=\left|\begin{matrix}[1^3]\\ w_1\end{matrix}\right\rangle\left|\begin{matrix}[3]\\ w_2\end{matrix}\right\rangle,\\
&\left|[1^3],\begin{matrix}[21]&[21]\\ w_1&w_2\end{matrix}\right\rangle=\frac{1}{\sqrt{2}}\left[\left|\begin{matrix}[21]\\ w_1\end{matrix}\right\rangle_1\left|\begin{matrix}[21]\\ w_2\end{matrix}\right\rangle_2-\left|\begin{matrix}[21]\\ w_1\end{matrix}\right\rangle_2\left|\begin{matrix}[21]\\ w_2\end{matrix}\right\rangle_1\right].
\end{aligned} \tag{7-109}$$

Here $m=1,2$ denotes the Young tableaux $\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}$ and $\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}$ respectively, and $\tilde{m}$ represents the conjugate Young tableau.

Example: Find the $SU_6\supset SU_3\times SU_2$ baryon wave functions in the flavor–spin space. We choose the isospin representation, $i=u,d,s$. Suppose we need to find the proton wave function with spin $\frac{1}{2}$ and projection $-\frac{1}{2}$, belonging to the 56-dimensional irrep $[\nu]=[3]$ of SU_6.

According to Table 7.5-2, the Weyl tableau of the proton is $\begin{array}{|c|c|}\hline u&u\\\hline d\\\cline{1-1}\end{array}$, and the Weyl tableau corresponding to spin 1/2 and projection $-1/2$ is $\begin{array}{|c|c|}\hline \alpha&\beta\\\hline \beta\\\cline{1-1}\end{array}$. Setting $w_1=\begin{array}{|c|c|}\hline u&u\\\hline d\\\cline{1-1}\end{array}$ and $w_2=\begin{array}{|c|c|}\hline \alpha&\beta\\\hline \beta\\\cline{1-1}\end{array}$ in the first equation of (7-109), we obtain the required wave function

$$\begin{aligned}
|[3],P_{1/2-1/2}\rangle&=\left|[3],\begin{array}{|c|c|}\hline u&u\\\hline d\\\cline{1-1}\end{array}\ \begin{array}{|c|c|}\hline \alpha&\beta\\\hline \beta\\\cline{1-1}\end{array}\right\rangle\\
&=\sqrt{\frac{1}{2}}\left(\left|\begin{array}{|c|c|}\hline u&u\\\hline d\\\cline{1-1}\end{array}\right\rangle_1\left|\begin{array}{|c|c|}\hline \alpha&\beta\\\hline \beta\\\cline{1-1}\end{array}\right\rangle_1+\left|\begin{array}{|c|c|}\hline u&u\\\hline d\\\cline{1-1}\end{array}\right\rangle_2\left|\begin{array}{|c|c|}\hline \alpha&\beta\\\hline \beta\\\cline{1-1}\end{array}\right\rangle_2\right).
\end{aligned} \tag{7-110a}$$

Using Tables 7.5-5 and 7.5-6, the above wave function can be expressed in terms of the product states

$$\begin{aligned}
|[3],P_{1/2-1/2}\rangle=\sqrt{\frac{1}{2}}\Big[&\frac{1}{6}(2|uud\rangle-|udu\rangle-|duu\rangle)(|\alpha\beta\beta\rangle+|\beta\alpha\beta\rangle-2|\beta\beta\alpha\rangle)\\
&+\frac{1}{2}(|udu\rangle-|duu\rangle)(|\alpha\beta\beta\rangle-|\beta\alpha\beta\rangle)\Big].
\end{aligned} \tag{7-110b}$$

We also have

$$|[3],\Delta^{+}_{3/2,1/2}\rangle = |[3]\,,\boxed{u}\boxed{u}\boxed{d}\;\boxed{\alpha}\boxed{\alpha}\boxed{\beta}\,\rangle = |\boxed{u}\boxed{u}\boxed{d}\,\rangle|\boxed{\alpha}\boxed{\alpha}\boxed{\beta}\,\rangle\ . \tag{7-110c}$$

Analogously, from the fourth equation of (7-109), we get the wave function for the excited states of the proton with spin $3/2$ and projection $-1/2$, belonging to the 70–dimensional irrep $[\nu]=[21]$ of SU_6

$$\Big|{}^{[21]}_{m,P_{3/2-1/2}}\Big\rangle = \Big|\begin{array}{|c|c|}\hline u&u\\\hline d\\\cline{1-1}\end{array}\Big\rangle_m|\boxed{\alpha}\boxed{\beta}\boxed{\beta}\,\rangle\ . \tag{7-111a}$$

Letting the tableau w_1 in (7-109) be $\begin{array}{|c|c|}\hline u&u\\\hline c\\\cline{1-1}\end{array}$, $\begin{array}{|c|c|}\hline u&s\\\hline c\\\cline{1-1}\end{array}$, and so on, we get the $SU_8 \supset SU_4 \times SU_2$ wave function. Thus we have

$$|[3],S^{+}_{1/2,1/2}\rangle = \sqrt{\frac{1}{2}}\left(\Big|\begin{array}{|c|c|}\hline u&s\\\hline c\\\cline{1-1}\end{array}\Big\rangle_1\Big|\begin{array}{|c|c|}\hline \alpha&\alpha\\\hline \beta\\\cline{1-1}\end{array}\Big\rangle_1 + \Big|\begin{array}{|c|c|}\hline u&s\\\hline c\\\cline{1-1}\end{array}\Big\rangle_2\Big|\begin{array}{|c|c|}\hline \alpha&\alpha\\\hline \beta\\\cline{1-1}\end{array}\Big\rangle_2\right)\ . \tag{7-111b}$$

In the above we considered only the wave function of the proton in flavor–spin space. In orbital space, the three constituent quarks of the proton, which is the ground state of the three–quark system, must be in the totally symmetric state $\psi^{[3]}(x)$. If there were no other degrees of freedom, the total wave function of the proton would be $\psi^{[3]}(x)\times|[3],P_{\frac{1}{2}S_z}\rangle$, which is totally symmetric. However, the quarks are assumed to be fermions, and the total wave function has to be anti–symmetric. To eliminate this contradiction, one assumes that the quark has a new degree of freedom, called the *color* degree of freedom. Besides flavor, a quark also has one of the three *colors*, red, green or blue, denoted by r,g,b. The quarks r,g and b carry the fundamental rep of the SU_3 group in color space. One also assumes that observable baryons and mesons are all colorless, that is, in the color singlet $|[0]\rangle^{(c)}$ of the color SU_3. For a three–quark system, the color singlet is

$$|[0]\rangle^{(c)} = |[1^3]\rangle^{(c)} = \left|\begin{array}{|c|}\hline r\\\hline g\\\hline b\\\hline\end{array}\right\rangle\ . \tag{7-112a}$$

Therefore, the totally anti–symmetric state of the proton is

$$|P_{\frac{1}{2}S_z}) = \psi^{[3]}(x)|[1^3]\rangle^{(c)}|[3],P_{\frac{1}{2}S_z}\rangle\ , \tag{7-112b}$$

while the totally anti–symmetric state of the particle Δ (the excited state of the nucleon) is

$$|\Delta_{\frac{3}{2}S_z}) = \psi^{[3]}(x)|[1^3]\rangle^{(c)}|[3],\Delta_{\frac{3}{2}S_z}\rangle. \tag{7-112c}$$

7.9.2. The irreps $([\nu_1],[\nu_2])$ of the groups SU_m and SU_2 contained in the irrep $[\nu]$ of SU_{mn}.

From (7-106) we know that the induction rule

$$([\nu_1]\times[\nu_2])\uparrow SU_{mn} = \sum_{\nu}(\nu_1\nu_2\nu)D^{[\nu]}(SU_{mn})\ , \tag{7-113a}$$

as well as the subduction rule

$$[\nu]\downarrow(SU_m\times SU_n) = \sum_{\nu}(\nu_1\nu_2\nu)(D^{[\nu_1]}(SU_m),D^{[\nu_2]}(SU_n))\ , \tag{7-113b}$$

are governed by the CG series of the permutation group, so long as we ignore the entire columns of length mn in the Young diagram $[\nu]$ of (7-113a), and entire columns of length $m(n)$ in the Young diagram $[\nu_1]([\nu_2])$ of (7-113b).

For example, from the CG series (Table 4.10) and (4-90), we find the irreps $[\nu_1]$ and $[\nu_2]$ of SU_3 and SU_2 contained in the irrep [3] and [21] of SU_6 as follows:

$$\begin{aligned}[3] \to &([3],[3]) + ([21],[21]) = ([3],[3]) + ([21],[1]) \ , \\ &\text{dimension: } 56 = (10,4) + (8,2) \ . \end{aligned} \tag{7-114a}$$

$$\begin{aligned}[21] \to &([3],[21]) + ([21],[3]) + ([21],[21]) + ([1^3],[21]) \\ &= ([3],[1]) + ([21],[3]) + ([21],[1]) + ([1^3],[1]) \ , \\ &\text{dimension: } 70 = (10,2) + (8,4) + (8,2) + (1,2) \ . \end{aligned} \tag{7-114b}$$

The equality of the dimensions offers a useful check for the correctness of the decomposition, as shown in Eq. (7-114).

7.9.3. Representation transformation between the $SU_{mn} \supset SU_m \times SU_n$ irreducible basis and the SU_{mn} Gel'fand basis

The $SU_{mn} \supset SU_m \times SU_n$ irreducible basis in (7-106a) is expressed in terms of the products of wave functions in x and ξ spaces. It can also be expressed in terms of the Gel'fand bases of SU_{mn} and the Yamanouchi bases of $S_f(q)$, $\left| \begin{matrix} [\nu] \\ m, W \end{matrix} \right\rangle$,

$$\left| \begin{matrix} [\nu] & \beta[\nu_1][\nu_2] \\ m, & w_1 \quad w_2 \end{matrix} \right\rangle = \sum_w \left| \begin{matrix} [\nu] \\ m, w \end{matrix} \right\rangle \left\langle \begin{matrix} [\nu] \\ w \end{matrix} \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1 w_2 \end{matrix} \Big\rangle \ . \tag{7-115}$$

The transformation coefficients, or the *subduction coefficients* (SDC) of $SU_{mn} \downarrow SU_m \times SU_n$, are obviously independent of m, therefore the label m in (7-115) can be ignored and (7-115) takes the following form,

$$\left| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1 w_2 \end{matrix} \right\rangle = \sum_w \left| \begin{matrix} [\nu] \\ w \end{matrix} \right\rangle \left\langle \begin{matrix} [\nu] \\ w \end{matrix} \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1 w_2 \end{matrix} \Big\rangle \ . \tag{7-116a}$$

The SU_{mn} SDC obey the unitarity relation

$$\sum_w \left\langle \begin{matrix} [\nu] \\ w \end{matrix} \right| [\nu] \ , \begin{matrix} \beta[\nu_1] & [\nu_2] \\ w_1 & w_2 \end{matrix} \Big\rangle \left\langle \begin{matrix} [\nu] \\ w \end{matrix} \right| [\nu] \ , \begin{matrix} \beta'[\nu_1'] & [\nu_2'] \\ w_1' & w_2' \end{matrix} \Big\rangle = \delta_{\beta\beta'} \delta_{\nu_1 \nu_1'} \delta_{w_1 w_1'} \delta_{w_2 w_2'} \ ,$$

$$\sum_{\beta \nu_1 \nu_2, w_1 w_2} \left\langle \begin{matrix} [\nu] \\ w \end{matrix} \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1 w_2 \end{matrix} \Big\rangle \left\langle \begin{matrix} [\nu] \\ w' \end{matrix} \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1 w_2 \end{matrix} \Big\rangle = \delta_{ww'} \ . \tag{7-116b}$$

The inverse of (7-116a) is

$$\left| \begin{matrix} [\nu] \\ w \end{matrix} \right\rangle = \sum_{\nu_1 \nu_2 \beta w_1 w_2} \left| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1 w_2 \end{matrix} \right\rangle \left\langle [\nu] \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1 w_2 \end{matrix} \Big\rangle \ . \tag{7-116c}$$

The SU_{mn} SDC in (7-115) can be found by using Racah's step operator method.

Ex. 7.8. Find the $SU_6 \supset SU_3 \times SU_2$ wave function $|[3], \Sigma^0_{\frac{1}{2}\frac{1}{2}}\rangle$.

Ex. 7.9. Find the $SU_3 \times SU_2$ content in the irrep [31] of SU_6.

7.10. The $SU_{n_1n_2n_3} \supset SU_{n_1} \times SU_{n_2} \times SU_{n_3}$ Irreducible Bases and the Racah Coefficients of Permutation Groups*

Suppose a particle has three kinds of degrees of freedom $x_i (i = 1, 2, 3)$. In the space V_{x_i} there are n_i single particle states. We have two ways to construct the $SU_n \supset SU_{n_1} \times SU_{n_2} \times SU_{n_3} (n = n_1 n_2 n_3)$ irreducible basis.

1. $SU_n \supset (SU_{n_1 n_2} \supset SU_{n_1} \times SU_{n_2}) \times SU_{n_3}$ basis. From (7-106a), this kind of basis can be expressed as

$$\left| \begin{matrix} [\nu] \\ m, \end{matrix} \left(\begin{matrix} [\nu_{12}] & [\nu_3] \\ [\nu_1]w_1[\nu_2]w_2, & w_3 \end{matrix} \right) \right\rangle^{\beta_{12}\beta} = \sum_{m_1 m_2 m_3 m_{12}} C^{[\nu_{12}]\beta_{12},m_{12}}_{\nu_1 m_1, \nu_2 m_2} C^{[\nu]\beta,m}_{[\nu_{12}]m_{12},[\nu_3]m_3} \left| \begin{matrix} [\nu_1] \\ m_1 w_1 \end{matrix} \right\rangle^{x_1} \left| \begin{matrix} [\nu_2] \\ m_2 w_2 \end{matrix} \right\rangle^{x_2} \left| \begin{matrix} [\nu_3] \\ m_3 w_3 \end{matrix} \right\rangle^{x_3}, \tag{7-117}$$

which is the Yamanouchi basis $[\nu]m$ of $S_f(q)$ with $q = (x_1, x_2, x_3)$, the irreducible basis $[\nu_i]w_i$ of SU_{n_i}, and belongs to the irreps $[\nu]$ and $[\nu_{12}]$ of SU_n and $SU_{n_1 n_2}$, respectively.

2. $SU_n \supset SU_{n_1} \times (SU_{n_2 n_3} \supset SU_{n_2} \times SU_{n_3})$ irreducible basis. Similarly we have

$$\left| \begin{matrix} [\nu] \\ m, \end{matrix} \left(\begin{matrix} [\nu_1] & [\nu_{23}] \\ w_1, & [\nu_2]w_2[\nu_3]w_3 \end{matrix} \right) \right\rangle^{\beta_{23}\beta'} = \sum_{m_1 m_2 m_3 m_{23}} C^{[\nu]\beta',m}_{\nu_1 m_1, \nu_{23} m_{23}} C^{[\nu_{23}]\beta_{23},m_{23}}_{\nu_2 m_2, \nu_3 m_3} \left| \begin{matrix} [\nu_1] \\ m_1 w_1 \end{matrix} \right\rangle^{x_1} \left| \begin{matrix} [\nu_2] \\ m_2 w_2 \end{matrix} \right\rangle^{x_2} \left| \begin{matrix} [\nu_3] \\ m_3 w_3 \end{matrix} \right\rangle^{x_3}, \tag{7-118}$$

which is the Yamanouchi basis $[\nu]m$ of $S_f(q)$, the irreducible basis $[\nu_i]w_i$ of SU_{n_i}, and belongs to the irreps $[\nu]$ and $[\nu_{23}]$ of SU_n and $SU_{n_2 n_3}$, respectively.

Suppose for instance that x_1 is the orbital space, $n_1 = 2l + 1$, and that x_2 and x_3 are spin and isospin spaces, $n_2 = n_3 = 2$. Using (7-118) and (4-124), a totally anti-symmetric state is constructed,

$$\left| [1^f] \left(\begin{matrix} [\nu_1] & [\nu_{23}] \\ w_1, & \beta[\nu_2]w_2[\nu_3]w_3 \end{matrix} \right) \right\rangle = \left| [1^f], \begin{matrix} [\nu_1] & [\tilde{\nu}_1] \\ \alpha LM, & \beta S M_S T M_T \end{matrix} \right\rangle = \sum_{m_1 m_2 m_3} \frac{\Lambda^{\nu_1}_{m_1}}{\sqrt{h_{\nu_1}(S_f)}} C^{[\tilde{\nu}_1]\beta,\tilde{m}_1}_{\nu_2 m_2, \nu_3 m_3} \left| \begin{matrix} [\nu_1] \\ m_1, \alpha LM \end{matrix} \right\rangle^{x_1} \left| \begin{matrix} [\nu_2] \\ m_2, \ S M_S \end{matrix} \right\rangle^{x_2} \left| \begin{matrix} [\nu_3] \\ m_3, \ T M_T \end{matrix} \right\rangle^{x_3} \tag{7-119}$$

where $\beta = \beta_{23}, [\nu_2] = [\frac{f}{2} + S, \frac{f}{2} - S], [\nu_3] = [\frac{f}{2} + T, \frac{f}{2} - T]$. Equation (7-119) is the $SU_{4(2l+1)} \supset SU_{2l+1} \times (SU_4 \supset SU_2 \times SU_2)$ basis.

DeGrand (1976) used the $SU_{12} \supset SU_3^f \times SU_2^s \times SU_2^p$ irreducible basis in the study of the bag model of elementary particles, where f, s and p stand for flavor, spin and pseudo-spin. Since the particles state must be a singlet $|[1^3]\rangle$ in color space, the irrep of SU_{12} is $[\nu] = [3]$, while $[\nu_1] = [\nu_2] = [\nu_3] = [21]$. Now the quantum numbers β, ν_{12} and β_{12} are redundant. From (7-117) and Table 4.13-1 we obtain the required wave function

$$\begin{aligned} \left| [\nu]; \ \begin{matrix} [\nu_1][\nu_2][\nu_3] \\ w_1 w_2 w_3 \end{matrix} \right\rangle &= \left| [3]; \begin{array}{|c|c|}\hline u & d \\ \hline s \\ \cline{1-1} \end{array} \begin{array}{|c|c|}\hline \alpha & \alpha \\ \hline \beta \\ \cline{1-1} \end{array} \begin{array}{|c|c|}\hline a & a \\ \hline b \\ \cline{1-1} \end{array} \right\rangle \\ &= \sum_{m_1 m_2 m} C^{[21],m}_{[21]m_1,[21]m_2} \left| \begin{array}{|c|c|}\hline u & d \\ \hline s \\ \cline{1-1} \end{array} \right\rangle_{m_1} \left| \begin{array}{|c|c|}\hline \alpha & \alpha \\ \hline \beta \\ \cline{1-1} \end{array} \right\rangle_{m_2} \left| \begin{array}{|c|c|}\hline a & a \\ \hline b \\ \cline{1-1} \end{array} \right\rangle_{m} \\ &= \frac{1}{2} \left[\left| \begin{array}{|c|c|}\hline u & d \\ \hline s \\ \cline{1-1} \end{array} \right\rangle_1 \left| \begin{array}{|c|c|}\hline \alpha & \alpha \\ \hline \beta \\ \cline{1-1} \end{array} \right\rangle_1 - \left| \begin{array}{|c|c|}\hline u & d \\ \hline s \\ \cline{1-1} \end{array} \right\rangle_2 \left| \begin{array}{|c|c|}\hline \alpha & \alpha \\ \hline \beta \\ \cline{1-1} \end{array} \right\rangle_2 \right] \left| \begin{array}{|c|c|}\hline a & a \\ \hline b \\ \cline{1-1} \end{array} \right\rangle_1 \\ &\quad - \frac{1}{2} \left[\left| \begin{array}{|c|c|}\hline u & d \\ \hline s \\ \cline{1-1} \end{array} \right\rangle_1 \left| \begin{array}{|c|c|}\hline \alpha & \alpha \\ \hline \beta \\ \cline{1-1} \end{array} \right\rangle_2 + \left| \begin{array}{|c|c|}\hline u & d \\ \hline s \\ \cline{1-1} \end{array} \right\rangle_2 \left| \begin{array}{|c|c|}\hline \alpha & \alpha \\ \hline \beta \\ \cline{1-1} \end{array} \right\rangle_1 \right] \left| \begin{array}{|c|c|}\hline a & a \\ \hline b \\ \cline{1-1} \end{array} \right\rangle_2, \end{aligned} \tag{7-120}$$

where a and b denote the pseudo–spin up and down states. Equation (7-120) is identical with DeGrand's result.

The bases of (7-117) and (7-118) differ by a unitary transformation

$$\left|\begin{matrix}[\nu]\\ m,\end{matrix}\left(\begin{matrix}[\nu_{12}] & [\nu_3]\\ [\nu_1]w_1[\nu_2]w_2, & w_3\end{matrix}\right)\right\rangle^{\beta_{12}\beta}$$

$$= \sum_{\nu_{23}\beta_{23}\beta'} U(\nu_1\nu_2\nu\nu_3, \nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'} \left|\begin{matrix}[\nu]\\ m,\end{matrix}\left(\begin{matrix}[\nu_1] & [\nu_{23}]\\ w_1, [\nu_2]\, w_2[\nu_3]w_3\end{matrix}\right)\right\rangle^{\beta_{23}\beta'}, \tag{7-121}$$

where U is the *Racah coefficient of the permutation group.* From (7-117) and (7-118) we have

$$U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'} = \sum_{\text{fix } m} C^{[\nu_{12}]\beta_{12},m_{12}}_{\nu_1 m_1,\nu_2 m_2} C^{[\nu]\beta,m}_{\nu_{12}m_{12},\nu_3 m_3} C^{[\nu_{23}]\beta_{23},m_{23}}_{\nu_2 m_2,\nu_3 m_3} C^{[\nu]\beta',m}_{\nu_1 m_1,\nu_{23}m_{23}}, \tag{7-122}$$

where the summation is over all the m_i's except m.

The values of U are independent of m, w_1, w_2 and w_3. If we ignore the unitary group and pay attention only to the permutation group, (7-121) can be written in the familiar form of angular momentum theory,

$$|([\nu_1][\nu_2])[\nu_{12}], [\nu_3] : [\nu]m\rangle^{\beta_{12}\beta}$$

$$= \sum_{\nu_{23}\beta_{23}\beta'} U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'} |[\nu_1]([\nu_2][\nu_3])[\nu_{23}] : [\nu]m\rangle^{\beta_{23}\beta'}. \tag{7-123}$$

Compared with the Racah coefficients of the group SU_2, the only difference here is the occurrence of the multiplicity labels $\beta_{12}, \beta_{23}, \beta$ and β' due to the non–simple reducibility of the permutation group. The Racah coefficients satisfy the unitarity relations

$$\sum_{\nu_{23}\beta_{23}\beta'} U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'} U(\nu_1\nu_2\nu\nu_3; \overline{\nu}_{12}\nu_{23})^{\overline{\beta}_{12}\overline{\beta}}_{\beta_{23}\beta'} = \delta_{\beta_{12}\overline{\beta}_{12}}\delta_{\beta\overline{\beta}}\delta_{\nu_{12}\overline{\nu}_{12}}, \tag{7-124a}$$

$$\sum_{\nu_{12}\beta_{12}\beta} U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'} U(\nu_1\nu_2\nu\nu_3; \nu_{12}\overline{\nu}_{23})^{\beta_{12}\beta}_{\overline{\beta}_{23}\overline{\beta}'} = \delta_{\beta_{23}\overline{\beta}_{23}}\delta_{\beta'\overline{\beta}'}\delta_{\nu_{23}\overline{\nu}_{23}}. \tag{7-124b}$$

The formulas in the SU_2 Racah algebra (Rose, 1957) can all be extended to the Racah coefficients of the permutation group. For example,

$$C^{[\nu_{12}]\beta_{12},m_{12}}_{\nu_1 m_1,\nu_2 m_3} C^{[\nu]\beta,m}_{\nu_{12}m_{12},\nu_3 m_3} = \sum_{\beta_{23}\beta'} U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'} C^{[\nu_{23}]\beta_{23},m_{23}}_{\nu_2 m_2,\nu_3 m_3} C^{[\nu]\beta',m}_{\nu_1 m_1,\nu_{23}m_{23}}, \tag{7-125}$$

$$\sum_{\beta'} U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'} C^{[\nu]\beta',m}_{\nu_1 m_1,\nu_{23}m_{23}} = \sum_{m_2 m_3 m_{12}} C^{[\nu_{12}]\beta_{12},m_{12}}_{\nu_1 m_1,\nu_2 m_2} C^{[\nu]\beta,m}_{\nu_{12}m_{12},\nu_3 m_3} C^{[\nu_{23}]\beta_{23},m_{23}}_{\nu_2 m_2,\nu_3 m_3}. \tag{7-126}$$

The generalized formulas of the SU_2 Racah algebra (Chen 1965) can also be extended to the permutation group. Letting

$$\{CCCC\} \equiv C^{[\nu_{12}]\beta_{12},m_{12}}_{\nu_1 m_1,\nu_2 m_2} C^{[\nu]\beta,m}_{\nu_{12}m_{12},\nu_3 m_3} C^{[\nu]\beta' m}_{\nu_1 m_1,\nu_{23}m_{23}} C^{[\nu_{23}]\beta_{23},m_{23}}_{\nu_2 m_2,\nu_3 m_3}, \tag{7-127}$$

equations (13) and (14) in Chen (1965) are generalized to

$$\sum_{\text{fix } m_\kappa} \{CCCC\} = \frac{h_\nu}{h_{\nu_\kappa}} U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'} \tag{7-128a}$$

$$\sum_{\text{fix } m_a m_b m_\kappa} \{CCCC\} \left\{C^{[\nu_\kappa]\beta_\kappa,m_\kappa}_{\nu_a m_a,\nu_b m_b}\right\}^{-1}$$

$$= \frac{h_\nu}{h_{\nu_\kappa}} \sum_{\beta_\kappa} C^{[\nu_\kappa]\beta_\kappa,m_\kappa}_{\nu_a m_a,\nu_b m_b} U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'}, \tag{7-128b}$$

where, the summation in (7-128a) is over all the m's except m_κ, while in (7-128b) over all the m's except m_a, m_b and m_κ. We use h_ν and h_{ν_κ} for the dimensions of the irreps $[\nu]$ and $[\nu_\kappa]$ of the permutation group, respectively. The value of $\nu_\kappa m_\kappa$ may be any one of $\nu_1 m_1, \nu_2 m_2, \nu_3 m_3, \nu_{12} m_{12}, \nu_{23} m_{23}$ and νm. The coefficient $C^{[\nu_\kappa]\beta_\kappa, m_\kappa}_{\nu_a m_a, \nu_b m_b}$ in (7-128b) may be any one of the four C's in (7-127).

Using (4-189a), the Racah coefficients of S_f can be expressed in terms of those of S_{f-1} and the $S_f \supset S_{f-1}$ ISF,

$$U(\nu_1\nu_2\nu\nu_3;\nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'} = \sum_{\substack{\nu'_1\nu'_2\nu'_3\nu'_{12}\nu'_{23} \\ \theta_{12}\theta_{23}\theta\theta'}} U(\nu'_1\nu'_2\nu'\nu'_3;\nu'_{12}\nu'_{23})^{\theta_{12}\theta}_{\theta_{23}\theta'}$$
$$\times C^{\nu_{12}\beta_{12},\nu'_{12}\theta_{12}}_{\nu_1\nu'_1,\nu_2\nu'_2} C^{\nu\beta,\nu'\theta}_{\nu_{12}\nu'_{12},\nu_3\nu'_3} C^{\nu_{23}\beta_{23},\nu'_{23}\theta_{23}}_{\nu_2\nu'_2,\nu_3\nu'_3} C^{\nu\beta',\nu'\theta'}_{\nu_1\nu'_1,\nu_{23}\nu'_{23}}, \tag{7-129}$$

where ν' and ν'_i refer to the group S_{f-1} and the summation is carried out with fixed ν'. From (7-126) we have

$$\sum_{\beta'} U(\nu_1\nu_2\nu\nu_3;\nu_{12}\nu_{23})^{\beta_{12}\beta}_{\beta_{23}\beta'} C^{\nu\beta',\nu'\theta'}_{\nu_1\nu'_1,\nu_{23}\nu'_{23}} = \sum_{\substack{\nu'_2\nu'_3\nu'_{12} \\ \theta_{12}\theta_{23}\theta}} U(\nu'_1\nu'_2\nu'\nu'_3;\nu'_{12}\nu'_{23})^{\theta_{12}\theta}_{\theta_{23}\theta'}$$
$$\times C^{\nu_{12}\beta_{12},\nu'_{12}\theta_{12}}_{\nu_1\nu'_1,\nu_2\nu'_2} C^{\nu\beta,\nu'\theta}_{\nu_{12}\nu'_{12},\nu_3\nu'_3} C^{\nu_{23}\beta_{23},\nu'_{23}\theta_{23}}_{\nu_2\nu'_2,\nu_3\nu'_3}. \tag{7-130}$$

Algebraic expressions have been given for some special Racah coefficients of the permutation group (Vanagas 1972).

7.11. The irreducible basis $\mathbf{SU}_{n_1n_2n_3n_4} \supset \mathbf{SU}_{n_1} \times \mathbf{SU}_{n_2} \times \mathbf{SU}_{n_3} \times \mathbf{SU}_{n_4}$ and the 9ν–Coefficients of the Permutation Group*

Let $n = n_1n_2n_3n_4$. There are two possible ways of constructing the SU_n irreducible basis.

1. The $SU_n \supset (SU_{n_1n_2} \supset SU_{n_1} \times SU_{n_2}) \times (SU_{n_3n_4} \supset SU_{n_3} \times SU_{n_4})$ irreducible basis.

$$\left| \begin{matrix} [\nu] \\ m \end{matrix}, \begin{pmatrix} [\nu_{12}] & [\nu_{34}] \\ [\nu_1]w_1[\nu_2]w_2, & [\nu_3]w_3[\nu_4]w_4 \end{pmatrix} \right\rangle^{\tau_{12}\tau_{34}\tau} = \sum_{\substack{m_1m_2m_3m_4 \\ m_{12}m_{34}}} C^{[\nu_{12}]\tau_{12},m_{12}}_{\nu_1m_1,\nu_2m_2} C^{[\nu_{34}]\tau_{34},m_{34}}_{\nu_3m_3,\nu_4m_4}$$
$$\times C^{[\nu]\tau,m}_{\nu_{12}m_{12},\nu_{34}m_{34}} \left| \begin{matrix} [\nu_1] \\ m_1w_1 \end{matrix} \right\rangle^{x_1} \left| \begin{matrix} [\nu_2] \\ m_2w_2 \end{matrix} \right\rangle^{x_2} \left| \begin{matrix} [\nu_3] \\ m_3w_3 \end{matrix} \right\rangle^{x_3} \left| \begin{matrix} [\nu_4] \\ m_4w_4 \end{matrix} \right\rangle^{x_4}. \tag{7-131}$$

2. The $SU_n \supset (SU_{n_1n_3} \supset SU_{n_1} \times SU_{n_3}) \times (SU_{n_2n_4} \supset SU_{n_2} \times SU_{n_4})$ irreducible basis

$$\left| \begin{matrix} [\nu] \\ m, \end{matrix} \begin{pmatrix} [\nu_{13}] & [\nu_{24}] \\ [\nu_1]w_1[\nu_3]w_3, & [\nu_2]w_2[\nu_4]w_4 \end{pmatrix} \right\rangle^{\tau_{13}\tau_{24}\tau'} = \sum_{\substack{m_1m_2m_3m_4 \\ m_{13}m_{24}}} C^{[\nu_{13}]\tau_{13},m_{13}}_{\nu_1m_1,\nu_3m_3} C^{[\nu_{24}]\tau_{24},m_{24}}_{\nu_2m_2,\nu_4m_4}$$
$$\times C^{[\nu]\tau',m}_{\nu_{13}m_{13},\nu_{24}m_{24}} \left| \begin{matrix} [\nu_1] \\ m_1w_1 \end{matrix} \right\rangle^{x_1} \left| \begin{matrix} [\nu_2] \\ m_2w_2 \end{matrix} \right\rangle^{x_2} \left| \begin{matrix} [\nu_3] \\ m_3w_3 \end{matrix} \right\rangle^{x_3} \left| \begin{matrix} [\nu_4] \\ m_4w_4 \end{matrix} \right\rangle^{x_4}. \tag{7-132}$$

The bases (7-131) and (7-132) are related by a unitary transformation

$$\left| \begin{matrix} [\nu] \\ m, \end{matrix} \begin{pmatrix} [\nu_{12}] & [\nu_{34}] \\ [\nu_1]w_1[\nu_2]w_2, & [\nu_3]w_3[\nu_4]w_4 \end{pmatrix} \right\rangle^{\tau_{12}\tau_{34}\tau}$$
$$= \sum_{\substack{\nu_{13}\nu_{24} \\ \tau_{13}\tau_{24}\tau'}} \begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ \nu_3 & \nu_4 & \nu_{34} \\ \nu_{13} & \nu_{24} & \nu \end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} \left| \begin{matrix} [\nu] \\ m \end{matrix}, \begin{pmatrix} [\nu_{13}] & [\nu_{24}] \\ [\nu_1]w_1[\nu_3]w_3, & [\nu_2]w_2[\nu_4]w_4 \end{pmatrix} \right\rangle^{\tau_{13}\tau_{24}\tau'}. \tag{7-133}$$

The coefficients in (7-133) are the 9ν–coefficients of the permutation group , and can be expressed as

$$\begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ \nu_3 & \nu_4 & \nu_{34} \\ \nu_{13} & \nu_{24} & \nu \end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} = \sum_{\text{fix } m} \{CCCCCC\} \,. \tag{7-134a}$$

$$\{CCCCCC\} = C^{[\nu_{12}]\tau_{12},m_{12}}_{\nu_1 m_1,\nu_2 m_2} C^{[\nu_{34}]\tau_{34},m_{34}}_{\nu_3 m_3,\nu_4 m_4} C^{[\nu]\tau,m}_{\nu_{12}m_{12},\nu_{34}m_{34}} C^{[\nu_{13}]\tau_{13},m_{13}}_{\nu_1 m_1,\nu_3 m_3} C^{[\nu_{24}]\tau_{24},m_{24}}_{\nu_2 m_2,\nu_4 m_4} \times C^{[\nu]\tau',m}_{\nu_{13}m_{13},\nu_{24}m_{24}} \,. \tag{7-134b}$$

Equations (9) and (10) in Chen (1965) can be extended to

$$\sum_{\text{fix } m_k} \{CCCCCC\} = \frac{h_\nu}{h_{\nu_k}} \begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ \nu_3 & \nu_4 & \nu_{34} \\ \nu_{13} & \nu_{24} & \nu \end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} \,. \tag{7-135a}$$

$$\sum_{\text{fix } m_a m_b m_k} \{CCCCCC\}\{C^{[\nu_k]\tau_k,m_k}_{\nu_a m_a,\nu_b m_b}\}^{-1} = \frac{h_\nu}{h_{\nu_k}} \sum_{\tau_k} C^{[\nu_k]\tau_k,m_k}_{\nu_a m_a,\nu_b m_b} \begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ \nu_3 & \nu_4 & \nu_{34} \\ \nu_{13} & \nu_{24} & \nu \end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} \,. \tag{7-135b}$$

The summation in (7-135a) is over all m's except m_k, while in (7-135b) the summation extends over all m's except m_a, m_b and m_k.

In analogy with (7-130), the 9ν coefficients of S_f are expressible in terms of those of S_{f-1} and the $S_f \supset S_{f-1}$ ISF,

$$\begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ \nu_3 & \nu_4 & \nu_{34} \\ \nu_{13} & \nu_{24} & \nu \end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} = \sum_{\text{fix } \nu'} \begin{pmatrix} \nu'_1 & \nu'_2 & \nu'_{12} \\ \nu'_3 & \nu'_4 & \nu'_{34} \\ \nu'_{13} & \nu'_{24} & \nu' \end{pmatrix}^{\theta_{12}\theta_{34}\theta}_{\theta_{13}\theta_{24}\theta'} C^{\nu_{12}\tau_{12},\nu'_{12}\theta_{12}}_{\nu_1\nu'_1,\nu_2\nu'_2} \times C^{\nu_{34}\tau_{34},\nu'_{34}\theta_{34}}_{\nu_3\nu'_3,\nu_4\nu'_4} C^{\nu\tau,\nu'\theta}_{\nu_{12}\nu'_{12},\nu_{34}\nu'_{34}} C^{\nu_{13}\tau_{13},\nu'_{13}\theta_{13}}_{\nu_1\nu'_1,\nu_3\nu'_3} C^{\nu_{24}\tau_{24},\nu'_{24}\theta_{24}}_{\nu_2\nu'_2,\nu_4\nu'_4} C^{\nu\tau',\nu'\theta'}_{\nu_{13}\nu'_{13},\nu_{24}\nu'_{24}} \,, \tag{7-136}$$

where the sum runs over $\nu'_1\nu'_2\nu'_3\nu'_4\nu'_{12}\nu'_{34}\nu'_{13}\nu'_{24}\theta_{12}\theta_{34}\theta_{13}\theta_{24}\theta\theta'$, but with ν' fixed. It is readily seen that

$$\begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ 0 & \nu_3 & \nu_3 \\ \nu_1 & \nu_{23} & \nu \end{pmatrix}^{\tau_{12}\tau}_{\tau_{23}\tau'} = U(\nu_1\nu_2\nu\nu_3;\nu_{12}\nu_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} \,. \tag{7-137}$$

The values of the 9ν coefficients are independent of $w_1w_2w_3w_4m$. If we are only interested in the permutation group, (7-133) can be written as

$$|(\nu_1\nu_2)\nu_{12},(\nu_3\nu_4)\nu_{34};\nu m)\rangle^{\tau_{12}\tau_{34}\tau} = \sum_{\tau_{13}\tau_{24}\tau'} \begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ \nu_3 & \nu_4 & \nu_{34} \\ \nu_{13} & \nu_{24} & \nu \end{pmatrix}^{\tau_{12}\tau_{34},\tau}_{\tau_{13}\tau_{24}\tau'} |(\nu_1\nu_3)\nu_{13},(\nu_2\nu_4)\nu_{24};\nu m\rangle^{\tau_{13}\tau_{24}\tau'} \,. \tag{7-138}$$

7.12. The $SU_{m+n} \supset SU_m \otimes SU_n$ Irreducible Basis

Suppose that there are two sets of single particle states with m and n states, and that there are f_1 and f_2 particles occupying the m states of the first set and the n states of the second set, respectively. For example, in the mixed configuration $(l_1)^{f_1}(l_2)^{f_2}$, there are f_1 particles in the orbital l_1 and f_2 particles in the orbital l_2; thus $m = 2l_1 + 1$ and $n = 2l_2 + 1$. Now we need to construct the $SU_{m+n} \supset SU_m \otimes SU_n$ irreducible bases for the $f_1 + f_2$ particles.

7.12.1. The IDC of permutation groups and the $SU_{m+n} \supset SU_m \otimes SU_n$ irreducible basis

We have three kinds of product states, $\varphi^{(1)}, \varphi^{(2)}$ and φ with particle numbers f_1, f_2 and $f = f_1 + f_2$, respectively:

$$\varphi^{(1)} = \varphi_{i_1}(1) \ldots \varphi_{i_{f_1}}(f_1), \quad i = 1, 2, \ldots, m \,. \tag{7-139a}$$

$$\varphi^{(2)} = \varphi_{j_1}(f_1 + 1) \ldots \varphi_{j_{f_2}}(f), \quad j = m+1, \ldots, m+n, f = f_1 + f_2 \,. \tag{7-139b}$$

$$\varphi = \varphi_{k_1}(1) \ldots \varphi_{k_f}(f), \quad k = 1, 2, \ldots, m+n \,. \tag{7-139c}$$

The $\begin{pmatrix} \varphi^{(1)} \\ \varphi^{(2)} \\ \varphi \end{pmatrix}$ carry a reducible rep of $\begin{pmatrix} S_{f_1} \\ S_{f_2} \\ S_f \end{pmatrix}$ and $\begin{pmatrix} SU_m \\ SU_n \\ SU_{m+n} \end{pmatrix}$. In the following we will use the symbol S_{f_2} to denote the permutation group $S_{f_2}(f_1 + 1, \ldots, f_1 + f_2)$.

The group elements of SU_m, SU_n, SU_{m+n} and $SU_m \otimes SU_n$ are of the following forms

$$\left(\begin{array}{c|c} U_0 & 0 \\ \hline 0 & I \end{array}\right), \quad \left(\begin{array}{c|c} I & 0 \\ \hline 0 & U_2 \end{array}\right), \quad \begin{pmatrix} u_{11} & \cdots & U_{1,m+n} \\ \vdots & & \vdots \\ u_{m+n,1} & \cdots & u_{m+n,m+n} \end{pmatrix}, \quad \left(\begin{array}{c|c} U_1 & 0 \\ \hline 0 & U_2 \end{array}\right). \tag{7-140}$$

Their orders are $r_m = m^2 - 1, r_n = n^2 - 1, r = (m+n)^2 - 1$ and $r' = r_m + r_n$, respectively. Evidently, $SU_m \otimes SU_n$ is a subgroup of SU_{m+n}. $\binom{\varphi^{(1)}}{\varphi^{(2)}}$ can be linearly combined into the Yamanouchi basis $\binom{(\nu_1 m_1)}{(\nu_2 m_2)}$ of $\binom{S_{f_1}}{S_{f_2}}$ and the Gel'fand basis $\binom{(\nu_1 w_1)}{(\nu_2 w_2)}$ of $\binom{SU_m}{SU_n}$, the Weyl tableaux w_1 and w_2 being filled with the state indices $i_1 \ldots i_f$ and $j_1 \ldots j_f$, respectively. The aforementioned bases are designated by

$$\left| \begin{matrix} [\nu_1] \\ m_1 \omega_1^0, w_1 \end{matrix} \right\rangle = \varphi_{m_1}^{[\nu_1]}(\omega_1^0, w_1) \,, \quad \left| \begin{matrix} [\nu_2] \\ m_2 \omega_2^0, w_2 \end{matrix} \right\rangle = \varphi_{m_2}^{[\nu_2]}(\omega_2^0, w_2) \,,$$

respectively. Using the IDC of permutation groups, they can be coupled into the Yamanouchi basis (νm) of S_f,

$$\begin{aligned} \left| \begin{matrix} [\nu] \\ m, \beta[\nu_1] w_1 [\nu_2] w_2 \end{matrix} \right\rangle &\equiv \left| \begin{matrix} [\nu], & \beta[\nu_1][\nu_2] \\ m & w_1 w_2 \end{matrix} \right\rangle \\ &= \sum_{\substack{m_1 \omega_1 \\ m_2 \omega_2}} C^{[\nu]\beta, m}_{\nu_1 m_1 \omega_1, \nu_2 m_2 \omega_2} \binom{\omega_0}{\omega} \left[\left| \begin{matrix} [\nu_1] \\ m_1 \omega_1^0, w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ m_2 \omega_2^0, w_2 \end{matrix} \right\rangle \right] \\ &= \sum_{\substack{m_1 \omega_1 \\ m_2 \omega_2}} C^{[\nu]\beta, m}_{\nu_1 m_1 \omega_1, \nu_2 m_2 \omega_2} \left| \begin{matrix} [\nu_1] \\ m_1 \omega_1, w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ m_2 \omega_2, w_2 \end{matrix} \right\rangle . \end{aligned} \tag{7-141a}$$

In analogy to the discussion following (7-106), it can be proved that (7-141a) belongs to the irrep $[\nu]$ of SU_{m+n}, and that it is also the irreducible basis $\nu_1 w_1 (\nu_2 w_2)$ of the group $SU_m(SU_n)$. Hence we have

Theorem 7.5: The IDC of permutation groups are the indirect coupling coefficients for the $SU_{m+n} \supset SU_m \otimes SU_n$ irreducible basis.

Therefore it is easy to construct the $SU_{m+n} \supset SU_m \otimes SU_n$ irreducible bases for arbitrary m and n by means of the IDC.

The inverse of (7-141a) is

$$\left| \begin{matrix} [\nu_1] \\ m_1 \omega_1, w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ m_2 \omega_2, w_2 \end{matrix} \right\rangle = \sum_{\nu \beta, m} C^{[\nu]\beta m}_{\nu_1 m_1 \omega_1, \nu_2 m_2 \omega_2} \left| \begin{matrix} [\nu], & \beta[\nu_1][\nu_2] \\ m & w_1 w_2 \end{matrix} \right\rangle . \tag{7-141b}$$

7.12.2. The content of irreps $([\nu_1],[\nu_2])$ of $SU_m \otimes SU_n$ in the irrep of SU_{m+n}

Equations (7-141) and (7-142) show that the SU_{m+n} subduction rule

$$[\nu] \downarrow (SU_m \otimes SU_n) = \sum_{\nu_1\nu_2} \{\nu_1\nu_2\nu\}(D^{[\nu_1]}(SU_m), D^{[\nu_2]}(SU_n)) \ , \tag{7-142a}$$

and the $SU_m \times SU_n$ induction rule

$$([\nu_1] \times [\nu_2]) \uparrow SU_{m+n} = \sum_{\nu} \{\nu_1\nu_2\nu\} D^{[\nu]}(SU_{m+n}) \ , \tag{7-142b}$$

are determined by the Littlewood rule, so long as we disregard the Young diagrams $[\nu_1]([\nu_2])$ of more than $m(n)$ rows and columns of length $m(n)$ in (7-142a), and the Young diagram $[\nu]$ of more than $m+n$ rows and columns of length $m+n$ in (7-142b).

For example, from Table 4.14-2 we obtain the irreps $([\nu_1],[\nu_2])$ of (SU_3, SU_2) contained in the irrep [32] of SU_5 as follows:

$$\begin{aligned} [32] \to\ & ([32],[0]) + ([0],[1]) + ([31],[1]) + ([1],[2]) \\ & + ([22],[1]) + ([1],[0]) + ([3],[2]) + ([2],[3]) \\ & + ([21],[2]) + ([2],[1]) + ([21],[0]) + ([11],[1]) \ , \\ \text{dimension } 175 \to\ & (15,1) + (1,2) + (15,2) + (3,3) + (6,2) + (3,1) \\ & + (10,3) + (6,4) + (8,3) + (6,2) + (8,1) + (3,2) \ . \end{aligned} \tag{7-143}$$

7.12.3. The representation transformation between the irreducible basis $SU_{m+n} \supset SU_m \otimes SU_n$ and the Gel'fand basis of SU_{m+n}

The $SU_{m+n} \supset SU_m \otimes SU_n$ irreducible bases (7-141a) can be expressed in terms of the SU_{m+n} Gel'fand bases:

$$\left| \begin{matrix} [\nu] \\ \beta[\nu_1][\nu_2]w_1[\nu_2]w_2 \end{matrix} \right\rangle = \left| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1\ w_2 \end{matrix} \right\rangle = \sum_w \left| \begin{matrix} [\nu] \\ w \end{matrix} \right\rangle \left\langle \begin{matrix} [\nu] \\ w \end{matrix} \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1\ w_2 \end{matrix} \Big\rangle \ . \tag{7-144}$$

The transformation coefficients $\left\langle \begin{matrix} [\nu] \\ w \end{matrix} \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1\ w_2 \end{matrix} \Big\rangle$, also known as the *subduction coefficients* (SDC) of $SU_{m+n} \downarrow SU_m \otimes SU_n$, also satisfy the unitarity relation (7-116), and are closely related to the SDC $\left\langle \begin{matrix} [\nu] \\ m \end{matrix} \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ m_1\ m_2 \end{matrix} \Big\rangle$ of the permutation group. Following the line of reasoning in Sec. 7.7 which led to (7-95), from (7-94) and (4-168a) we obtain

$$\begin{aligned} & \left| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1\ w_2 \end{matrix} \right\rangle R^{[\nu_1]m_1}(\overline{\omega}^0_1) R^{[\nu_2]m_2}(\overline{\omega}^0_2) \\ & \quad = \sum_m \left| \begin{matrix} [\nu] \\ w \end{matrix} \right\rangle R^{[\nu]m}(\overline{\omega}^0) \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ m_1\ m_2 \end{matrix} \Big\rangle \ . \end{aligned} \tag{7-145}$$

Comparing (7-144) with (7-145), we obtain a relation between the two coefficients,

$$\begin{aligned} & \left\langle \begin{matrix} [\nu] \\ w \end{matrix} \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ w_1\ w_2 \end{matrix} \Big\rangle \\ & \quad = \left[R^{[\nu_1]m_1}(\overline{\omega}^0_1) R^{[\nu_2]m_2}(\overline{\omega}^0_2) \right]^{-1} \sum_m{}' R^{[\nu]m}(\overline{\omega}^0) \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \right| [\nu], \begin{matrix} \beta[\nu_1][\nu_2] \\ m_1\ m_2 \end{matrix} \Big\rangle \ , \end{aligned} \tag{7-146a}$$

where $(\overline{\omega}^0), (\overline{\omega}_1^0)$ and $(\overline{\omega}_2^0)$ are the normal order states in the Weyl tableaux w, w_1 and w_2, respectively, that is, the Young tableaux $Y_m^{[\nu]}(\overline{\omega}^0), Y_{m_1}^{[\nu_1]}(\overline{\omega}_1^0)$ and $Y_{m_2}^{[\nu_2]}(\overline{\omega}_2^0)$ in state space. The prime in the summation symbol indicates that the sum is restricted to those m which give rise to the same Weyl tableau w.

Equation (7-146a) shows that once the SDC of the permutation group are known, the SDC of SU_{m+n} can be found for arbitrary m and n. Again, the values of the SU_{m+n} SDC do not depend on m and n explicitly.

In the case when the single particle states in the Weyl tableau w are all different, only one term survives in the summation of (7-146a) and all the normalization constants R become unity; hence

$$\left\langle \begin{matrix}[\nu] \\ w\end{matrix} \middle| [\nu], \begin{matrix}\beta[\nu_1][\nu_2] \\ w_1\ w_2\end{matrix} \right\rangle = \left\langle \begin{matrix}[\nu] \\ m\end{matrix} \middle| [\nu], \begin{matrix}\beta[\nu_1][\nu_2] \\ m_1\ m_2\end{matrix} \right\rangle. \tag{7-146b}$$

For example, by letting the ordinals 1,2,3,4 in the Young tableaux of Table 4.18 be the state indices $\alpha, \beta, \gamma, \delta$, respectively, the Young tableaux become the Weyl tableaux and the S_f SDC $\left\langle \begin{matrix}[\nu] \\ m\end{matrix} \middle| [\nu], \begin{matrix}\beta[\nu_1][\nu_2] \\ m_1\ m_2\end{matrix} \right\rangle$ become the SU_{m+n} SDC $\left\langle \begin{matrix}[\nu] \\ w\end{matrix} \middle| [\nu], \begin{matrix}\beta[\nu_1][\nu_2] \\ w_1\ w_2\end{matrix} \right\rangle$ such as

$$\left| [31], \boxed{\alpha}\ \begin{matrix}\boxed{\beta}\boxed{\gamma} \\ \boxed{\delta}\end{matrix} \right\rangle = \frac{\sqrt{8}}{3} \left| \begin{matrix}\boxed{\alpha}\boxed{\beta}\boxed{\gamma} \\ \boxed{\delta}\end{matrix} \right\rangle - \frac{1}{6} \left| \begin{matrix}\boxed{\alpha}\boxed{\beta}\boxed{\delta} \\ \boxed{\gamma}\end{matrix} \right\rangle - \frac{1}{\sqrt{12}} \left| \begin{matrix}\boxed{\alpha}\boxed{\gamma}\boxed{\delta} \\ \boxed{\beta}\end{matrix} \right\rangle .$$

Following the steps similar to those for calculating the SU_n CG coefficients from the permutation group IDC, we can obtain the SU_{m+n} SDC from the permutation group SDC by using (7-146a) and the normalization coefficients given in Table 4.8.

Thus by letting $(\omega^0) = (\alpha\beta\beta\delta)$ in Table 4.18-1, the Young tableaux in Table 4.18-1 become the Weyl tableaux in Table 7.12-1. It is seen that there are two β's in the tableau w_2 at the third row, thus

$$\left| [31]\ ,\ \boxed{\alpha}\ \begin{matrix}\boxed{\beta}\boxed{\gamma} \\ \boxed{\delta}\end{matrix} \right\rangle = 0\ .$$

Dividing the first and second rows of Table 4.18-1 by $R^{[3]}(\beta\beta\delta) = \sqrt{2}$ and $R^{[21]1}(\beta\beta\delta) = \sqrt{2}$, respectively, and multiplying the first, second and third columns of Table 4.18-1 by, respectively, $R^{[31]1}(\alpha\beta\beta\delta) = \sqrt{2}$, $R^{[31]2}(\alpha\beta\beta\delta) = \sqrt{\frac{1}{2}}$, and $R^{[31]3}(\alpha\beta\beta\delta) = \sqrt{\frac{3}{2}}$, we obtain Table 7.12-1. On adding the second and third columns which have the same heading, we obtain the SU_{m+n} SDC shown in Table 7.12-2.

Table 7.12-1. (Intermediate step)

	$\begin{matrix}\boxed{\alpha}\boxed{\beta}\boxed{\beta} \\ \boxed{\delta}\end{matrix}$	$\begin{matrix}\boxed{\alpha}\boxed{\beta}\boxed{\delta} \\ \boxed{\beta}\end{matrix}$	$\begin{matrix}\boxed{\alpha}\boxed{\beta}\boxed{\delta} \\ \boxed{\beta}\end{matrix}$
$[31], \boxed{\alpha}\ \boxed{\beta}\boxed{\beta}\boxed{\delta}$	$-\frac{1}{3}$	$-\frac{\sqrt{2}}{6}$	$-\frac{\sqrt{2}}{2}$
$[31], \boxed{\alpha}\ \begin{matrix}\boxed{\beta}\boxed{\beta} \\ \boxed{\delta}\end{matrix}$	$\frac{\sqrt{8}}{3}$	$-\frac{1}{12}$	$-\frac{1}{4}$
$[31], \boxed{\alpha}\ \begin{matrix}\boxed{\beta}\boxed{\delta} \\ \boxed{\beta}\end{matrix}$	0	0	0

Table 7.12-2. $\left\langle \begin{matrix}[\nu] \\ w\end{matrix} \middle| [\nu], \begin{matrix}[\nu_1]\ [\nu_2] \\ w_1\ w_1\end{matrix} \right\rangle$

	$\begin{matrix}\boxed{\alpha}\boxed{\beta}\boxed{\beta} \\ \boxed{\delta}\end{matrix}$	$\begin{matrix}\boxed{\alpha}\boxed{\beta}\boxed{\delta} \\ \boxed{\beta}\end{matrix}$
$[31], \boxed{\alpha}\ \boxed{\beta}\boxed{\beta}\boxed{\delta}$	$-\frac{1}{3}$	$-\frac{\sqrt{8}}{3}$
$[31], \boxed{\alpha}\ \begin{matrix}\boxed{\beta}\boxed{\beta} \\ \boxed{\delta}\end{matrix}$	$\frac{\sqrt{8}}{3}$	$-\frac{1}{3}$

Furthermore, by letting the normal order state $(\overline{\omega}^0) = (\alpha\beta\beta\delta)$ in Table 7.11-2 be equal to other possible states, we obtain the SDC for arbitrary SU_{m+n}. This is illustrated by setting

$$(\overline{\omega}_0) = (\alpha\beta\beta\delta) = (1223), (1224), (1225), (1334), (1335),$$
$$(1445), (2334), (2335), (2445), (3445)$$

we obtain the SDC of SU_5. Consequently, each SDC table gives an infinite number of coefficients with the same structure. The SU_{m+n} SDC are tabulated in Chen, Wang, Lü & Wu (1987).

7.13. The Isoscalar Factors and the Fractional Parentage Coefficients

We use the round brackets, (|, or |), to denote a antisymmetric state in the total space, while the ordinary bracket, ⟨ |, or | ⟩ for states in partial space.

7.13.1. Isoscalar factors

1. The Gel'fand basis. The factorization formula (3-303) of the CG coefficients also applies to the Lie group. Since the Gel'fand basis is the $SU_n \supset SU_{n-1} \otimes U_1 \supset \ldots \supset SU_2 \otimes U_1 \supset SO_2$ irreducible basis, its CG coefficients can be decomposed into a product of a set of $SU_i \supset SU_{i-1} \times U_1$ ISF (summing over the intermediate multiplicity labels, if there are any). The $SU_i \supset SU_{i-1} \times U_1$ ISF is also called the SU_{i-1} *singlet factor*, abbreviated as SU_{i-1} SF. Thus the CG coefficients of SU_n for the Gel'fand basis can be expressed schematically as

$$(SU_n \text{ CGC}) = (SU_{n-1} \text{ SF})(SU_{n-2} \text{ SF}) \ldots (SU_2 \text{ SF})(SU_2 \text{ CGC}) \,. \tag{7-147}$$

The SU_2 CG coefficients are just the SU_1 SF. Therefore the evaluation of the CG coefficients of SU_n is reduced to the evaluation of SU_i SF. From (3-303) we get:

Example 1: The CG coefficients of SU_3:

$$C^{[\mu]\theta,IYI_z}_{[\mu_1]I_1Y_1I_{1z},[\mu_2]I_2Y_2I_{2z}} = C^{[\mu]\theta,IY}_{[\mu_1]I_1Y_1,[\mu_2]I_2Y_2} C^{I,I_z}_{I_1I_{1z},I_2I_{2z}} \tag{7-148}$$

SU_3 CGC $\qquad$ SU_2 SF $\qquad$ SU_2 CGC

Example 2: The CG coefficients of SU_4:

$$C^{[\nu]\tau,[\mu]ZIYI_z}_{[\nu_1][\mu_1]Z_1I_1Y_1I_{1Z},[\nu_2][\mu_2]Z_2I_2Y_2I_{2Z}} = \sum_\theta C^{[\nu]\tau,[\mu]_\theta Z}_{[\nu_1][\mu_1]Z_1,[\nu_2][\mu_2]Z_2} C^{[\mu]\theta,IY}_{[\mu_1]I_1Y_1,[\mu_2]I_2Y_2} C^{I,I_z}_{I_1I_{1z},I_2I_{2z}} \,. \tag{7-149}$$

SU_3 SF $\qquad$ SU_2 SF $\qquad$ SU_2 CGC

Tables of the SU_2 SF and SU_3 SF are given by de Swart (1963) and Haacke (1976), respectively. A new method for calculating the SU_nSF will be given in Sec. 7.17.

2. The $SU_{mn} \supset SU_m \times SU_n$ and $SU_{m+n} \supset SU_m \otimes SU_n$ irreducible bases. Both irreducible bases will be designated by

$$\left| \begin{matrix} [\nu] \\ \beta[\sigma]w_1[\mu]w_2 \end{matrix} \right\rangle, \quad \begin{matrix} \beta = 1,2,\ldots,(\nu_1\nu_2\nu) \text{ for } SU_{mn} \,, \\ \beta = 1,2,\ldots,\{\nu_1\nu_2\nu\} \text{ for } SU_{m+n} \,, \end{matrix} \tag{7-150}$$

where ν, σ and μ are the irrep labels for SU_{mn} (or SU_{m+n}), SU_m and SU_n, respectively.

Setting $\Lambda = [\sigma][\mu], m = w_1w_2$ in (3-300) we get

$$\left| \begin{matrix} [\nu]\tau \\ \beta[\sigma]w_1[\mu]w_2 \end{matrix} \right\rangle = \sum C^{[\nu]\tau,\beta[\sigma][\mu]w_1w_2}_{[\nu']\beta'\sigma'\mu'w_1'w_2',[\nu'']\beta''\sigma''\mu''w_1''w_2''} \times \left| \begin{matrix} [\nu'] \\ \beta'[\sigma']w_1'[\mu']w_2' \end{matrix} \right\rangle \left| \begin{matrix} [\nu''] \\ \beta''[\sigma'']w_1''[\mu'']w_2'' \end{matrix} \right\rangle , \tag{7-151}$$

where the sum runs over $\beta'\sigma'\mu'w_1'w_2'\beta''\sigma''\mu''w_1''w_2''$. Analogously, by index substitution, from (3-303) we obtain the factorization formula for the $SU_{mn}(SU_{m+n})$ CG coefficients

$$C^{[\nu]\tau,\beta[\sigma][\mu]w_1w_2}_{[\nu']\beta'\sigma'\mu'w_1'w_2',[\nu'']\beta''\sigma''\mu''w_1''w_2''} = \sum_{\theta\varphi} C^{[\nu]\tau,\beta[\sigma]_\theta[\mu]_\varphi}_{[\mu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} C^{[\sigma]\theta,w_1}_{\sigma'w_1'\sigma''w_1''} C^{[\mu]\varphi,w_2}_{\mu'w_2',\mu''w_2''} \,,$$
$$\theta = 1,2,\ldots,\{\sigma'\sigma''\sigma\} \,, \quad \varphi = 1,2,\ldots,\{\mu'\mu''\mu\} \,. \tag{7-152}$$

The first factor on the right-hand side is the $SU_{mn} \supset SU_m \times SU_n$ or $SU_{m+n} \supset SU_m \otimes SU_n$ ISF, and the second and third factors are the SU_m and SU_n CG coefficients, respectively. Equation (7-152) can be expressed schematically as

$$\begin{aligned}(SU_{mn} \supset SU_m \times SU_n \text{ CGC}) &= (SU_{mn} \supset SU_m \times SU_n \text{ ISF})(SU_m \text{ CGC})(SU_n \text{ CGC}),\\ (SU_{m+n} \supset SU_m \otimes SU_n \text{ CGC}) &= (SU_{m+n} \supset SU_m \otimes SU_n \text{ ISF})(SU_m \text{ CGC})(SU_n \text{ CGC})\ .\end{aligned} \tag{7-153}$$

By index substitutions in (3-305) and (3-306), we obtain the unitarity relation of the ISF. For fixed $[\sigma]$ and $[\mu]$ we have

$$\sum_{\substack{\beta'\sigma'\mu'\theta\\ \beta''\sigma''\mu''\varphi}} C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'[\sigma'][\mu'],[\nu'']\beta''[\sigma''][\mu'']} C^{[\overline{\nu}]\overline{\tau},\overline{\beta}[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'[\sigma'][\mu'],[\nu'']\beta''[\sigma''][\mu'']} = \delta_{\nu\overline{\nu}}\delta_{\beta\overline{\beta}}\delta_{\tau\overline{\tau}}\ , \tag{7-154a}$$

$$\begin{aligned}&\sum_{\nu\beta\tau} C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'[\sigma'][\mu'],[\nu'']\beta''[\sigma''][\mu'']} C^{[\nu]\tau,\beta[\sigma]\overline{\theta}[\mu]\overline{\varphi}}_{[\nu']\overline{\beta}'[\overline{\sigma}'][\overline{\mu}'],[\nu'']\overline{\beta}''[\overline{\sigma}''][\overline{\mu}'']}\\ &\quad = \delta_{\beta'\overline{\beta}'}\delta_{\beta''\overline{\beta}''}\delta_{\sigma'\overline{\sigma}'}\delta_{\sigma''\overline{\sigma}''}\delta_{\mu'\overline{\mu}'}\delta_{\mu''\overline{\mu}''}\delta_{\theta\overline{\theta}}\delta_{\varphi\overline{\varphi}}\ .\end{aligned} \tag{7-154b}$$

The calculation methods for the $SU_{mn} \supset SU_m \times SU_n$ and $SU_{m+n} \supset SU_m \otimes SU_n$ ISF are given in Sec. 7.16 and Sec. 7.17.

Example 3: The $SU_4 \supset SU_2 \times SU_2$ ISF. Now the multiplicity labels θ and φ are redundant, and the irreps of SU_2 are labelled by the spin S or isospin T. Equation (7-152) takes the following form:

$$C^{[\nu]\tau,\beta STM_S M_T}_{[\nu_1]\beta_1 S_1 T_1 M_{S_1} M_{T_1},[\nu_2]\beta_2 S_2 T_2 M_{S2} M_{T2}} = C^{[\nu]\tau,\beta ST}_{[\nu_1]\beta_1 S_1 T_1,[\nu_2]\beta_2 S_2 T_2} C^{SM_S}_{S_1 M_{S_1},S_2 M_{S_2}} C^{TM_T}_{T_1 M_{T_1},T_2 M_{T_2}}\ . \tag{7-155}$$

Example 4: The $SU_6 \supset SU_3 \times SU_2$ ISF. $[\nu]$, $[\mu]$ and S are used to label the irreps of SU_6, SU_3 and SU_2, respectively. The $SU_6 \supset SU_3 \times SU_2$ CG coefficients are expressed as

$$\begin{aligned}&C^{[\nu]\tau,\beta[\mu]IYSI_z S_z}_{[\nu_1]\beta_1[\mu_1]I_1 Y_1 S_1 I_{1z} S_{1z},[\nu_2]\beta_2[\mu_2]I_2 Y_2 S_2 I_{2z} S_{2z}}\\ &\quad = \sum_{\theta} C^{[\nu]\tau,\beta[\mu]\theta S}_{[\nu_1]\beta_1[\mu_1]S_1,[\nu_2]\beta_2[\mu_2]S_2} C^{[\mu]x\theta,IYI_z}_{[\mu_1]I_1 Y_1 I_{1z},[\mu_2]I_2 Y_2 I_{2z}} C^{S,S_z}_{S_1 S_{1z} S_2 S_{2z}}\ .\end{aligned} \tag{7-156}$$

Example 5: The $SU_{2l+1} \supset SO_3$ ISF. The $SU_{2l+1} \supset SO_3$ irreducible basis is denoted by $\left|\begin{matrix}[\nu]\\ \alpha LM\end{matrix}\right\rangle$, where α distinguishes multiple occurrences of the irrep L of SO_3 in the irrep $[\nu]$ of SU_{2l+1}. We have

$$\begin{aligned}&C^{[\nu]\tau,\alpha LM}_{[\nu_1]\alpha_1 L_1 M_1,[\nu_2]\alpha_2 L_2 M_2} = C^{[\nu]\tau,\alpha L}_{[\nu_1]\alpha_1 L_1,[\nu_2]\alpha_2 L_2} C^{LM}_{L_1 M_1,L_2 M_2}\ .\\ &SU_{2l+1} \supset SO_3 \text{ CGC}, \qquad SU_{2l+1} \supset SO_3 \text{ ISF}, SO_3 \text{ CGC}\end{aligned} \tag{7-157}$$

Equations (3-302) and (3-307) now take the following form:

$$\left|\begin{matrix}[\nu]\tau\\ \alpha LM\end{matrix}\right\rangle = \sum_{\alpha_1 L_1 \alpha_2 L_2} C^{[\nu]\tau,\alpha L}_{[\nu_1]\alpha_1 L_1,[\nu_2]\alpha_2 L_2} \left[\left|\begin{matrix}[\nu_1]\\ \alpha_1 L_1\end{matrix}\right\rangle \left|\begin{matrix}[\nu_2]\\ \alpha_2 L_2\end{matrix}\right\rangle\right]^L_M\ , \tag{7-158a}$$

$$\left[\left|\begin{matrix}[\nu_1]\\ \alpha_1 L_1\end{matrix}\right\rangle \left|\begin{matrix}[\nu_2]\\ \alpha_2 L_2\end{matrix}\right\rangle\right]^L_M = \sum_{\nu\tau\alpha} C^{[\nu]\tau,\alpha L}_{[\nu_1]\alpha_1 L_1,[\nu_2]\alpha_2 L_2} \left|\begin{matrix}[\nu]\tau\\ \alpha LM\end{matrix}\right\rangle\ , \tag{7-158b}$$

where the square brackets denote angular momentum coupling.

7.13.2. The orbital fractional parentage coefficients (CFP)

1. *The single particle CFP.*

Suppose that there are $n-1$ particles in the orbital l and they are in a state $\left| \begin{matrix} l^{n-1}[\nu_1] \\ m_1, \alpha_1 L_1 M_1 \end{matrix} \right\rangle$, which is the Yamanouchi basis $[\nu_1]m_1$ of S_{n-1} and the $SU_{2l+1} \supset SO_3$ irreducible basis $\left| \begin{matrix} [\nu_1] \\ \alpha_1 L_1 M_1 \end{matrix} \right\rangle$. Our aim is to construct a similar state $\left| \begin{matrix} l^n[\nu] \\ m, \alpha L M \end{matrix} \right\rangle$ for the n–particle system. Since $\left| \begin{matrix} l^{n-1}[\nu_1] \\ m_1, \alpha_1 L_1 M_1 \end{matrix} \right\rangle \times \psi_{lm_l}(n)$ form a complete set, we have

$$\left| \begin{matrix} l^n[\nu] \\ m, \alpha L M \end{matrix} \right\rangle = \sum_{\alpha_1 L_1} \langle l^{n-1}[\nu_1]\alpha_1 L_1, l|\}l^n[\nu]\alpha L\rangle \left[\left| \begin{matrix} l^{n-1}[\nu_1] \\ m_1, \alpha_1 L_1 \end{matrix} \right\rangle \psi_l(n) \right]^L_M . \tag{7-159a}$$

The coefficients $(l^{n-1}[\nu_1]\alpha_1 L_1, l|\}l^n[\nu]\alpha L)$ appearing in the above expression are called the *orbital one-particle CFP*. The name derives from the fact that each state of the $n-1$ particles can be considered as a fractional parent of the n-particle state. The quantum number $\nu_1 m_1$ and νm are related by $[\nu]m = [\nu][\nu_1]m_1$, in other words, the tableaux resulting from the deletion of the last box in $Y^{[\nu]}_m$, is $Y^{[\nu_1]}_{m_1}$.

On the other hand, according to (7-158a), we can use the $SU_{2l+1} \supset SO_3$ ISF to couple $\left| \begin{matrix} l^{n-1}[\nu_1] \\ m_1 \alpha_1 L_1 \end{matrix} \right\rangle$ and $\psi^{[1]}_{lm_l}(n)$ into another $SU_{2l+1} \supset SO_3$ irreducible basis,

$$\left| \begin{matrix} l^n[\nu] \\ m, \alpha L M \end{matrix} \right\rangle = \sum_{\alpha_1 L_1} C^{[\nu]\alpha L}_{[\nu_1]\alpha_1 L_1, [1]l} \left[\left| \begin{matrix} l^{n-1}[\nu_1] \\ m_1, \alpha_1 L_1 \end{matrix} \right\rangle \psi^{[1]}_l(n) \right]^L_M . \tag{7-159b}$$

Since the ISF are independent of the quantum numbers m_1 and M, (7-159b) can be simply written as

$$|[\nu]\alpha L\rangle = \sum_{\alpha_1 L_1} C^{[\nu]\alpha L}_{[\nu_1]\alpha_1 L_1, [1]l} |[\nu_1]\alpha_1 L_1\rangle \psi(n) , \tag{7-159c}$$

where the symbol, $[\ ]^L_M$, for angular momentum coupling is omitted. Examples of (7-159c) are given in (7-191) and (7-197).

From the definition of ISF, the left–hand side of (7-159b) must belong to the irrep $[\nu]$ of SU_{2l+1}, which by Theorem 7.1 implies that it also belongs to the irrep $[\nu]$ of S_n. In addition, once the quantum numbers $[\nu], [\nu_1]$ and $[m_1]$ are given, the quantum number m is also fixed. Therefore the left–hand side of (7-159b) is the Yamanouchi basis $[\nu]m$. Comparing (7-159a) with (7-159b) we see that the the one-particle orbital CFP is just the $SU_{2l+1} \supset SO_3$ ISF,

$$\langle l^{n-1}[\nu_1]\alpha_1 L_1, l|\}l^n[\nu]\alpha L\rangle = C^{[\nu],\alpha L}_{[\nu_1]\alpha_1 L_1, [1]l} . \tag{7-160}$$

They satisfy the unitarity relations

$$\sum_{\alpha_1 L_1} C^{[\nu],\alpha L}_{[\nu_1]\alpha_1 L_1 [1]l} C^{[\nu']\alpha' L}_{[\nu_1]\alpha_1 L_1, [1]l} = \delta_{\nu\nu'}\delta_{\alpha\alpha'} , \tag{7-161a}$$

$$\sum_{\nu\alpha} C^{[\nu],\alpha L}_{[\nu_1]\alpha_1 L_1, [1]l} C^{[\nu],\alpha L}_{[\nu_1]\alpha'_1 L'_1, [1]l} = \delta_{\alpha_1\alpha'_1}\delta_{L_1 L'_1} . \tag{7-161b}$$

The inverse of (7-159b) is

$$\left[\left| \begin{matrix} l^{n-1}[\nu_1] \\ m_1, \alpha_1 L_1 \end{matrix} \right\rangle \psi_l(n) \right]^L_M = \sum_{\nu\alpha} C^{[\nu],\alpha L}_{[\nu_1]\alpha_1 L_1, [1]l} \left| \begin{matrix} l^n[\nu] \\ m, \alpha L M \end{matrix} \right\rangle . \tag{7-162}$$

Between the groups SU_{2l+1} and SU_3, we often insert the subgroup SO_{2l+1} which contains SO_3 as its subgroup, and whose irrep label may serve as the additional label α. For example, for the d shell, one usually uses the $SU_5 \supset SO_5 \supset SO_3$ irreducible basis,

$$\left| \begin{matrix} d^n[\nu] \\ m,(\omega)LM \end{matrix} \right\rangle = \sum_{\omega_1 L_1} C^{[\nu],(\omega)L}_{[\nu_1](\omega_1)L_1,[1](\omega_2)d} \left[\left| \begin{matrix} d^{n-1}[\nu_1] \\ m_1,(\omega_1)L_1 \end{matrix} \right\rangle \psi_d(n) \right]^L_M , \tag{7-163}$$

where (ω) is the irrep label of SO_5. The first factor on the right-hand side of (7-163) is the $SU_5 \supset SO_5 \supset SO_3$ ISF which can be factorized as

$$C^{[\nu],(\omega)L}_{[\nu_1](\omega_1)L_1,[1](\omega_2)d} = C^{[\nu],(\omega)}_{[\nu_1](\omega_1),[1](\omega_2)} C^{(\omega),L}_{(\omega_1)L_1,(\omega_2)d} . \tag{7-164}$$

Further discussion can be found in Jahn (1950, 1951).

The definition of ISF can be extended to the mixed configuration case, such as the $2s, 1d$ shell. In analogy with (7-163), Elliott's $SU_6 \supset SU_3 \supset SO_3$ irreducible basis (Elliott 1958) is now expressed as

$$\begin{aligned} \left| \begin{matrix} [\nu] \\ m,\beta(\lambda\mu)KLM \end{matrix} \right\rangle = & \sum_{\beta_1 \lambda_1 \mu_1 K_1 L_1 L_2} C^{[\nu],\beta(\lambda\mu)}_{[\nu_1]\beta_1(\lambda_1\mu_1),[1](20)} \\ & \times C^{(\lambda\mu),KL}_{(\lambda_1\mu_1)K_1L_1,(20)L_2} \left[\left| \begin{matrix} [\nu_1] \\ m_1,\beta_1(\lambda_1\mu_1)K_1L_1 \end{matrix} \right\rangle \psi_{L_2}(n) \right]^L_M , \end{aligned} \tag{7-165}$$

where $[\nu], (\lambda\mu)$ are the irrep labels of SU_6 and SU_3, respectively, $L_2 = 0, 2$. The first and second factors in (7-165) are the $SU_6 \supset SU_3$ and $SU_3 \supset SO_3$ ISF, respectively. Notice that a single particle in the $2s, 1d$ shell belongs to the irrep (20) of SU_3.

2. *Many-particle CFP*

We now consider the CFP for separating n_2 particles from an n-particle system. We still use the symbols $(\omega_1^0) = (1, 2, \ldots, n_1)$ and $(\omega_2^0) = (n_1 + 1, \ldots, n), n = n_1 + n_2$, and use the $SU_{2l+1} \supset SO_3$ classification scheme as an example. The generalization to other group chains is straightforward.

The $S_n \supset S_{n_1} \otimes S_{n_2}$ and $SU_{2l+1} \supset SO_3$ irreducible basis can be expanded in terms of the $SU_{2l+1} \supset SO_3$ ISF,

$$\left| \begin{matrix} [\nu] \\ \tau\nu_1 m_1 \nu_2 m_2, \alpha L \end{matrix} \right\rangle = \sum_{\alpha_1 L_1 \alpha_2 L_2} C^{[\nu]\tau,\alpha L}_{\nu_1 \alpha_1 L_1, \nu_2 \alpha_2 L_2} \left[\left| \begin{matrix} l^{n_1}[\nu_1] \\ m_1\omega_1^0, \alpha_1 L_1 \end{matrix} \right\rangle \left| \begin{matrix} l^{n_2}[\nu_2] \\ m_2\omega_2^0, \alpha_2 L_2 \end{matrix} \right\rangle \right]^L , \tag{7-166a}$$

where the first factor on the right-hand side of (7-166a) is the $SU_{2l+1} \supset SO_3$ ISF, and is also called the many-particle CFP (Jahn, Elliott), and often written as

$$\langle l^{n_1}[\nu_1]\alpha_1 L_1, l^{n_2}[\nu_2]\alpha_2 L_2 | \} l^n[\nu]\tau\alpha L \rangle = C^{[\nu]\tau,\alpha L}_{\nu_1\alpha_1 L_1, \nu_2\alpha_2 L_2} . \tag{7-166b}$$

If the Yamanouchi basis is used, we have

$$\left| \begin{matrix} l^n[\nu] \\ m, \alpha L \end{matrix} \right\rangle = \sum \langle l^{n_1}[\nu_1]\alpha_1 L_1, l^{n_2}[\nu_2]\alpha_2 L_2 | \} l^n[\nu]\alpha L \rangle^{\nu'\nu''\ldots} \left[\left| \begin{matrix} l^{n_1}[\nu_1] \\ m_1\omega_1^0, \alpha_1 L_1 \end{matrix} \right\rangle \left| \begin{matrix} l^{n_2}[\nu_2] \\ m_2\omega_2^0, \alpha_2 L_2 \end{matrix} \right\rangle \right]^L \tag{7-167a}$$

where the sum runs over to $\nu_2 m_2 \alpha_1 L_1 \alpha_2 L_2$, and

$$\langle l^{n_1}[\nu_1]\alpha_1 L_1, l^{n_2}[\nu_2]\alpha_2 L_2 | \} l^n[\nu]\alpha L \rangle^{\nu'\nu''\ldots} = \sum_\tau \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \middle| [\nu], \begin{matrix} \tau\nu_1\nu_2 \\ m_1 m_2 \end{matrix} \right\rangle C^{[\nu]\tau,\alpha L}_{\nu_1\alpha_1 L_1, \nu_2\alpha_2 L_2} , \tag{7-167b}$$

is defined as the *many-particle CFP* in Kramer & Moshinsky 1968, which depends on the irrep labels $[\nu'], [\nu''], \ldots$ of the groups $S_{n-1}, S_{n-2}, \ldots S_{n-n_2+1}$ (due to the fact that $[\nu]m = [\nu][\nu'][\nu''] \ldots [\nu_1]m_1$). These two definitions of the CFP become identical for the one-body CFP. Both definitions of the CFP are discussed in this section, and they are distinguishable according to whether they carry the intermediate quantum numbers $\nu' \ldots$ or not.

In summary, the so-called CFP in the definition (7-166b) is either an ISF or a certain kind of CG coefficients. For instance the two-particle orbital CFP given by Harvey (1981, Table 4) are just the well known SU_2 coefficients.

3. *The two-particle CFP.*

Letting $n_2 = 2$ in (7-167a) and ignoring $[\nu_2]$ (= [2] or [11]), which is determined by the value of L_2, we have

$$\left| \begin{matrix} l^n[\nu] \\ m, \alpha L \end{matrix} \right\rangle = \sum_{\alpha_1 L_1 L_2} \langle l^{n-2}[\nu_1]\alpha_1 L_1, l^2 L_2 | \} l^n[\nu]\alpha L \rangle^{\nu'} \left[\left| \begin{matrix} l^{n-2}[\nu_1] \\ m_1\omega_1^0, \alpha_1 L_1 \end{matrix} \right\rangle \left| \begin{matrix} l^2 \\ \omega_2^0, L_2 \end{matrix} \right\rangle \right]^L . \quad (7\text{-}168a)$$

The two-particle CFP can be expressed in terms of the one-particle CFP. Using (7-159b) twice and the recoupling technique we have

$$\langle l^{n-2}[\nu_1]\alpha_1 L_1, l^2 L_2 | \} l^n[\nu]\alpha L \rangle^{\nu'} = \sum_{\alpha' L'} C^{[\nu],\alpha L}_{[\nu']\alpha' L',[1]l} C^{[\nu'],\alpha' L'}_{[\nu_1]\alpha_1 L_1,[1]l} U(L_1 l L l; L' L_2) . \quad (7\text{-}168b)$$

Extensions to other group chains is straightforward.

7.13.3. The spin-isospin CFP

1. *One-particle CFP.*

As was the case with (7-159b), one has

$$\left| \begin{matrix} \gamma^n[\tilde{\nu}] \\ \tilde{m}, \beta S T M_S M_T \end{matrix} \right\rangle = \sum_{\beta_1 S_1 T_1} C^{[\tilde{\nu}],\beta S T}_{[\tilde{\nu}_1]\beta_1 S_1 T_1,[1]\frac{1}{2}\frac{1}{2}} \left[\left| \begin{matrix} \gamma^{n-1}[\tilde{\nu}_1] \\ \tilde{m}_1, \beta_1 S_1 T_1 \end{matrix} \right\rangle \psi_{\frac{1}{2}\frac{1}{2}}(n) \right]^{ST}_{M_S M_T} . \quad (7\text{-}169a)$$

Equation (7-169a) is the Yamanouchi basis $[\tilde{\nu}]\tilde{m}$ of S_n and the $SU_4 \supset SU_2 \times SU_2$ irreducible basis $[\tilde{\nu}]ST$. The one-body spin-isospin CFP is just the $SU_4 \supset SU_2 \times SU_2$ ISF, and is usually designated by

$$\langle \gamma^{n-1}[\tilde{\nu}_1]\beta_1 S_1 T_1, \gamma | \} \gamma^n[\tilde{\nu}]\beta S T \rangle = C^{[\tilde{\nu}],\beta S T}_{[\tilde{\nu}_1]\beta_1 S_1 T_1,[1]\frac{1}{2}\frac{1}{2}} . \quad (7\text{-}169b)$$

2. *Two-particle CFP.*

Analogously to (7-168a), one has

$$\left| \begin{matrix} [\tilde{\nu}] \\ \tilde{m}, \beta S T M_S M_T \end{matrix} \right\rangle = \sum_{\beta_1 S_1 T_1 S_2 T_2} \langle \gamma^{n-2}[\tilde{\nu}_1]\beta_1 S_1 T_1,\ \gamma^2 S_2 T_2 | \} \gamma^n[\tilde{\nu}]\beta S T \rangle^{\tilde{\nu}'} \left[\left| \begin{matrix} \gamma^{n-2}[\tilde{\nu}_1] \\ \tilde{m}_1\omega_1^0, \beta_1 S_1 T_1 \end{matrix} \right\rangle \left| \begin{matrix} \gamma^2 \\ \omega_2^0, S_2 T_2 \end{matrix} \right\rangle \right]^{ST}_{M_S M_T} . \quad (7\text{-}170a)$$

The two-particle CFP are

$$\begin{aligned} &\langle \gamma^{n-2}[\tilde{\nu}_1]\beta_1 S_1 T_1,\ \gamma^2 S_2 T_2 | \} \gamma^n[\tilde{\nu}]\beta S T \rangle^{\tilde{\nu}'} \\ &= \left\langle \begin{matrix} [\tilde{\nu}] \\ \tilde{m} \end{matrix} \middle| [\tilde{\nu}],\ \begin{matrix} [\tilde{\nu}_1][\tilde{\nu}_2] \\ \tilde{m}_1 \end{matrix} \right\rangle C^{[\tilde{\nu}],ST}_{[\tilde{\nu}_1]\beta_1 S_1 T_1,[\tilde{\nu}_2] S_2 T_2} \\ &= \sum_{\beta' S' T'} C^{[\tilde{\nu}],\beta S T}_{[\tilde{\nu}']\beta' S' T',[1]\frac{1}{2}\frac{1}{2}} C^{[\tilde{\nu}'],\beta' S' T'}_{[\tilde{\nu}_1]\beta_1 S_1 T_1,[1]\frac{1}{2}\frac{1}{2}} U\left(S_1 \tfrac{1}{2} S \tfrac{1}{2}; S' S_2\right) U\left(T_1 \tfrac{1}{2} T \tfrac{1}{2}; T' T_2\right) . \end{aligned} \quad (7\text{-}170b)$$

7.13.4. The total CFP

We first discuss the CFP in the definition of Jahn and Elliott. Starting from (7-108), and making use of (4-168b), (4-180a) and (4-171b), the totally anti-symmetric wave function for n particles can be expressed as

$$\left|\begin{matrix} l^n[\nu] \\ \alpha\beta LSTM_SM_T \end{matrix}\right\rangle = \sum_{\tau\nu_1m_1\nu_2m_2} \varepsilon_3(\nu_1\nu_2\nu_\tau)\frac{\Lambda^{\nu_1}_{m_1}\Lambda^{\nu_2}_{m_2}}{\sqrt{h_\nu}} \left|\begin{matrix} l^n[\nu] \\ \tau\nu_1m_1\nu_2m_2, \alpha LM \end{matrix}\right\rangle \times \left|\begin{matrix} \gamma^n[\tilde{\nu}] \\ \tau\tilde{\nu}_1\tilde{m}_1\tilde{\nu}_2\tilde{m}_2, \beta STM_SM_T \end{matrix}\right\rangle . \tag{7-171}$$

Substituting (7-166a) and its counterpart in the spin-isospin space into (7-171), we get

$$\left|\begin{matrix} \rho^n[\nu] \\ \alpha\beta LSTMM_SM_T \end{matrix}\right\rangle = \sum_{\nu_1\Gamma_1\nu_2\Gamma_2} (\rho^{n-n_2}[\nu_1]\Gamma_1, \rho^{n_2}[\nu_2]\Gamma_2|\}\rho^n[\nu]\Gamma) \times \left[\left|\begin{matrix} \rho^{n-n_2}[\nu_1] \\ \alpha_1\beta_1L_1S_1T_1 \end{matrix}\right\rangle_{\omega_1^0} \left|\begin{matrix} \rho^{n_2}[\nu_2] \\ \alpha_2\beta_2L_2S_2T_2 \end{matrix}\right\rangle_{\omega_2^0}\right]^{LST}_{MM_SM_T} , \tag{7-172}$$

where $\rho = lst$, $\Gamma = \alpha L\beta ST$. The *total CFP* for separating n_2 particles out of n particles is

$$(\rho^{n-n_2}[\nu_1]\Gamma_1, \rho^{n_2}[\nu_2]\Gamma_2|\}\rho^n[\nu]\Gamma) = \sqrt{\frac{h_{\nu_1}h_{\nu_2}}{h_\nu}} \sum_\tau \varepsilon_3(\nu_1\nu_2\nu_\tau)\langle\rho^{n-n_2}[\nu_1]\Gamma_1, \rho^{n_2}[\nu_2]\Gamma_2|\}\rho^n[\nu]\tau\Gamma\rangle , \tag{7-173a}$$

$$\langle\rho^{n-n_2}[\nu_1]\Gamma_1, \rho^{n_2}[\nu_2]\Gamma_2|\}\rho^n[\nu]_\tau\Gamma\rangle = C^{[\nu]\tau,\alpha L}_{[\nu_1]\alpha_1L_1,[\nu_2]\alpha_2L_2} C^{[\tilde{\nu}]\tau,\beta ST}_{[\tilde{\nu}_1]\beta_1S_1T_1,[\tilde{\nu}_2]\beta_2S_2T_2} , \tag{7-173b}$$

where $(h_{\nu_1}h_{\nu_2}/h_\nu)^{\frac{1}{2}}$ is called the weight factor. As will be shown in (7-244b), $\varepsilon_3(\nu_1\nu_2\nu_\tau)\sqrt{\frac{h_{\nu_1}h_{\nu_2}}{h_\nu}}$ is the $SU_{4(2l+1)} \supset SU_{2l+1} \times SU_4$ ISF. Therefore, the so-called total CFP is precisely the $SU_{4(2l+1)} \supset (SU_{2l+1} \supset SO_3) \times (SU_4 \supset SU_2 \times SU_2)$ ISF,

$$(\rho^{n-n_2}[\nu_1]\Gamma_1, \rho^{n_2}[\nu_2]\Gamma_2|\}\rho^n[\nu]\Gamma) = C^{[1^n],[\nu]\alpha L[\tilde{\nu}]\beta ST}_{[1^{n_1}][\nu_1]\alpha_1L_1[\tilde{\nu}_1]\beta_1S_1T_1,[1^{n_2}][\nu_2]\alpha_2L_2[\tilde{\nu}_2]\beta_2S_2T_2} , \tag{7-174}$$

and we can use Racah's factorization lemma (3-303) to write down the expression (7-173) directly without the foregoing step-by-step derivation. Further discussion of the total CFP will be given in Sec. 7.16.5.

Next we turn to the CFP in the definition of Kramer & Moshinsky (1968). Starting from (7-108), using (7-159a) and (7-169a) for one-body case, (7-167a) and (7-170a) for two-body case, as well as (4-196') we can derive

$$|\rho^n[\nu]\Gamma) = \sum_{\nu_1\nu'\Gamma_1\Gamma_2} (\rho^{n-n_2}[\nu_1]\Gamma_1, \rho^{n_2}\Gamma_2|\}\rho^n[\nu]\Gamma)^{\nu'} \left[|\rho^{n-n_2}[\nu_1]\Gamma_1)|\rho^{n_2}\Gamma_2)\right]^\Gamma , \tag{7-175a}$$

where the redundant quantum number $[\nu_2]$ is omitted, the quantum number ν' should be ignored when $n_2 = 1$, and

$$(\rho^{n-1}[\nu_1]\Gamma_1, \rho|\}\rho^n[\nu]\Gamma) = \Lambda^\nu_{\nu_1}\sqrt{\frac{h_{\nu_1}}{h_\nu}}\langle\rho^{n-1}[\nu_1]\Gamma_1, \rho|\}\rho^n[\nu]\Gamma\rangle , \tag{7-175b}$$

$$\langle\rho^{n-1}[\nu_1]\Gamma_1, \rho|\}\rho^n[\nu]\Gamma\rangle = C^{[\nu],\alpha L}_{[\nu_1]\alpha_1L_1,[1]} C^{[\tilde{\nu}],\beta ST}_{[\tilde{\nu}_1]\beta_1S_1T_1,[1]} , \tag{7-175c}$$

$$(\rho^{n-2}[\nu_1]\Gamma_1, \rho^2\Gamma_2|\}\rho^n[\nu]\Gamma)^{\nu'} = \Lambda^{\nu}_{\nu'}\Lambda^{\nu'}_{\nu_1}\sqrt{\frac{h_{\nu_1}}{h_\nu}}\langle\rho^{n-n_2}[\nu_1]\Gamma_1, \rho^{n_2}\Gamma_2|\}\rho^n[\nu]\Gamma\rangle^{\nu'}$$
$$= \sum_{\Gamma'}(\rho^{n-2}[\nu_1]\Gamma_1, \rho|\}\rho^{n-1}[\nu']\Gamma')(\rho^{n-1}[\nu']\Gamma', \rho|\}\rho^n[\nu]\Gamma)U(\Gamma_1\rho\Gamma\rho;\Gamma'\Gamma_2)\ , \tag{7-175d}$$

$$\langle\rho^{n-n_2}[\nu_1]\Gamma_1, \rho^{n_2}\Gamma_2|\}\rho^n[\nu]\Gamma\rangle^{\nu'}$$
$$= \langle l^{n-2}[\nu_1]\alpha_1 L_1, l^2 L_2|\}l^n[\nu]\alpha L\rangle^{\nu'}\langle\gamma^{n-2}[\tilde{\nu}_1]\beta_1 S_1 T_1,\ \gamma^2 S_2 T_2|\}\gamma^n[\tilde{\nu}]\beta ST\rangle^{\tilde{\nu}'}, \tag{7-175e}$$

where

$$U(\Gamma_1\rho\Gamma\rho;\Gamma'\Gamma_2) = U(L_1 l L l; L' L_2)U(S_1\tfrac{1}{2}S\tfrac{1}{2}; S' S_2)U(T_1\tfrac{1}{2}T\tfrac{1}{2}; T' T_2). \tag{7-175f}$$

Equation (7-175d) is to be compared with (4.45) in Brussaard & Glaudemans 1977.

Due to $\varepsilon_3([\nu_1][1][\nu]) = \Lambda^{\nu}_{\nu_1}$ (see (4-180c)), The one-body total CFP's in (7-173a) and (7-175b) are the same, while the relation between the two-body total CFP's in the two definitions is obtained by comparing (7-172) and (7-175a),

$$(\rho^{n-2}[\nu_1]\Gamma_1, \rho^2\Gamma_2|\}\rho^n[\nu]\Gamma) = \sum_{\nu'}(\rho^{n-2}[\nu_1]\Gamma_1, \rho^2\Gamma_2|\}\rho^n[\nu]\Gamma)^{\nu'}\ . \tag{7-176}$$

From (7-168b) and (7-170b) it is seen that the two–body CFP in the Definition of Kramer & Moshinsky 1968 can be calculated from the one–body CFP's without a knowledge of the SDC of permutation group and is thus simpler and will be used henceforth.

7.13.5. The CFP for j–j coupling .

For the j–j coupling, the $[SU_{2l+1} \supset SO_{2l+1} \supset SO_3] \times SU_4$ group chain is replaced by $[SU_{2j+1} \supset Sp_{2j+1} \supset SO_3] \times SU_2$, with the quantum numbers as (see (9-58g))

$$\begin{array}{llllll} SU_{2N} \supset & [SU_N \supset & Sp_N \supset & SO_3] & \otimes & SU_2 \\ [1^n] & [\tilde{\nu}_T] & \beta(v\tau) & \alpha J & & T \end{array} \tag{7-177}$$

where $(v\tau)$ is the irrep label of Sp_N, and $[\tilde{\nu}_T] = \left[2^{\frac{n}{2}-T}, 1^{2T}\right]$

Equations (7-159)–(7-176) apply to the j–j coupling as well with the interpretation

$$\rho \to jt, \quad \Gamma \to \alpha JT, \quad l \to j, \quad L \to J, \quad (s,t) \to (0,t), \quad \beta(S,T) \to (0,T)$$

where α should be understood as the set of quantum numbers $\alpha\beta(v\tau)$ in (7-177).

According to (7-169) (ignoring s and S), the one-body CFP in isospin space is unit,

$$C^{[\tilde{\nu}],T}_{[\tilde{\nu}_1]T_1,[1]} = 1\ , \quad \text{if } [\tilde{\nu}_1]\otimes[1] \to [\tilde{\nu}]\ . \tag{7-178a}$$

The two-body isospin CFP can be obtained from (7-170b), (7-178a) and the fact that T' is related to $[\tilde{\nu}'] = \left[\frac{n}{2} - T', 2T'\right]$,

$$\langle t^{n-2}[\tilde{\nu}_1]T_1,\ t^2 T_2|\}t^n[\tilde{\nu}]T\rangle^{\tilde{\nu}'} = U(T_1\tfrac{1}{2}T\tfrac{1}{2}; T' T_2)\ . \tag{7-178b}$$

The one-body total CFP in (7-175b,c) become

$$(\rho^{n-1}[\nu_1]\alpha_1 J_1 T_1, \rho|\}\rho^n[\nu]\alpha JT) = \Lambda^{\nu}_{\nu_1}\sqrt{\frac{h_{\nu_1}}{h_\nu}}C^{[\nu],\alpha J}_{[\nu_1]\alpha_1 J_1,[1]j}\ , \tag{7-179}$$

The factor $\Lambda^{\nu}_{\nu_1}\sqrt{\frac{h_{\nu_1}}{h_\nu}}$ is the $SU_{2N} \supset SU_N \times SU_2$ ISF $C^{[1^n],\nu\tilde{\nu}}_{[1^{n-1}]\nu_1\tilde{\nu}_1,[1]}$ (see (7-232)), and can be expressed in terms of the number of particles, isospins T and T_1,

$$\Lambda^{\nu}_{\nu_1}\sqrt{\frac{h_{\nu_1}}{h_\nu}} = \begin{cases} \left[\frac{(T+1)(n-2T)}{n(2T+1)}\right]^{1/2}(-1)^n, & T_1 = T + \frac{1}{2} \\ \left[\frac{T(n+2T+2)}{n(2T+1)}\right]^{1/2}, & T_1 = T - \frac{1}{2} \end{cases} \tag{7-180}$$

The two-body total CFP is

$$(\rho^{n-2}[\nu_1]\alpha_1 J_1 T_1, \rho^2 J_2 T_2|\}\rho^n[\nu]\alpha JT)^{\nu'}$$
$$= \Lambda^{\nu}_{\nu'}\Lambda^{\nu'}_{\nu_1}\sqrt{\frac{h_{\nu_1}}{h_\nu}}\langle j^{n-2}[\nu_1]\alpha_1 J_1,\ j^2 J_2|\}j^n[\nu]\alpha J\rangle^{\nu'} U(T_1 \tfrac{1}{2} T \tfrac{1}{2}; T' T_2)\ . \tag{7-181}$$

For further discussion, see DeShalit (1963).

7.13.6. The eigenfunction method for evaluating the CFP

Several methods are available for evaluating the CFP or ISF. Here we introduce only the EFM. We first change notation and rewrite (7-159b) as

$$\psi\begin{pmatrix}[\nu]\\ m,\ \alpha L\end{pmatrix} = \sum_{\alpha_1 L_1} C^{[\nu],\alpha L}_{[\nu_1]\alpha_1 L_1,[1]}\left[\psi\begin{pmatrix}[\nu_1]\\ m_1,\ \alpha_1 L_1\end{pmatrix}\psi_l(n)\right]^L_M\ , \tag{7-182}$$

which is already the Yamanouchi basis $[\nu_1]m_1$ of S_{n-1}. Therefore the requirement for it to be the Yamanouchi basis $[\nu]m$ of S_n is equivalent to the requirement that it be an eigenfunction of the 2-cycle class operator $C(n)$ of S_n. In analogy to (4-191), we find the eigenequation satisfied by $\psi\begin{pmatrix}[\nu]\\ m,\alpha L\end{pmatrix}$ to be

$$C'(n)\psi\begin{pmatrix}[\nu]\\ m,\ \alpha L\end{pmatrix} = (\nu - \nu_1)\psi\begin{pmatrix}[\nu]\\ m,\ \alpha L\end{pmatrix}\ , \tag{7-183}$$

$$C'(n) = \sum_{i=1}^{n-1} p_{in}\ . \tag{7-184}$$

Consequently, to obtain the CFP $C^{[\nu]\alpha L}_{[\nu_1]\alpha_1 L_1,[1]}$, one only needs to diagonalize the operator $C'(n)$ in the basis $\left[\psi\begin{pmatrix}[\nu_1]\\ m_1,\alpha_1 L_1\end{pmatrix}\psi_l(n)\right]^L_M$ with fixed ν_1, m_1 and L. To obtain the matrix elements of $C'(n)$, we use (7-159) to expand the wave functions of $n-1$ particles. The matrix elements of the transposition $p_{n,n-1}$ are expressed as[3)]

$$\left\langle\left[\psi\begin{pmatrix}[\nu_1]\\ m_1,\alpha_1 L_1\end{pmatrix}\psi_l(n)\right]^L_M\middle|P_{n,n-1}\middle|\left[\psi\begin{pmatrix}[\nu_1]\\ m_1',\alpha_2 L_2\end{pmatrix}\psi_l(n)\right]^L_M\right\rangle$$
$$= \delta_{m_1 m_1'}\sum_{\alpha' L'} C^{[\nu_1],\alpha_1 L_1}_{[\nu']\alpha' L',[1]} C^{[\nu_1],\alpha_2 L_2}_{[\nu']\alpha' L',[1]}\langle L' L_1 L|p_{n,n-1}|L' L_2 L\rangle$$
$$= \delta_{m_1 m_1'}\langle\alpha_1 L_1|p_{n,n-1}|\alpha_2 L_2\rangle^{(L)}_{\nu_1 m_1}, \tag{7-185}$$

where $|L' L_1 L\rangle$ is shorthand for

$$|L' L_1 L\rangle = \left[\left[\psi\begin{pmatrix}[\nu']\\ m',\alpha' L'\end{pmatrix}\psi_l(n-1)\right]^{L_1}\psi_l(n)\right]^L\ . \tag{7-186}$$

[3)] When $[\nu_1]\neq[\nu_1']$, the matrix elements

$$\left\langle[\psi\begin{pmatrix}[\nu_1]\\ m_1,\alpha_1 L_1\end{pmatrix}\psi_l(n)]^L_M\middle|p_{n,n-1}\middle|[\psi\begin{pmatrix}[\nu_1']\\ m_1',\alpha_2 L_2\end{pmatrix}\psi_l(n)]^L_M\right\rangle$$
$$= \textstyle\sum_{\alpha' L'} C^{[\nu_1]\alpha_1 L_1}_{[\nu']\alpha' L',[1]} C^{[\nu_1']\alpha_2 L_2}_{[\nu']\alpha' L',[1]}\left\langle L' L_1 L|p_{n,n-1}|L' L_2 L\right\rangle$$

do not vanish for $m_1 \neq m_1'$, see Jahn (1951, Sec. 5).

It can be shown that

$$\langle L'L_1L|p_{n,n-1}|L'L_2L\rangle = (-1)^{L'+L+L_1+L_2}U(lL'Ll;L_1L_2)\ . \tag{7-187a}$$

$$\begin{aligned}\langle \alpha_1 L_1|p_{n,n-1}|\alpha_2 L_2\rangle^{(L)}_{\nu_1 m_1} &= \langle \alpha_2 L_2|p_{n,n-1}|\alpha_1 L_1\rangle^{(L)}_{\nu_1 m_1}\\ &= \sum_{\alpha' L'} C^{[\nu_1],\alpha_1 L_1}_{[\nu']\alpha' L',[1]} C^{[\nu_1],\alpha_2 L_2}_{[\nu']\alpha' L',[1]} \langle L'L_1L|p_{n,n-1}|L'L_2L\rangle\ .\end{aligned} \tag{7-187b}$$

(Numerical tables of $\langle L'L_1L|p_{n,n-1}|L'L_2L\rangle$ for $l = 1$ are given by Jahn 1951.) Using $p_{in} = p_{i,n-1}p_{n-1,n}p_{i,n-1}$ and (7-185) one gets

$$\begin{aligned}\langle \alpha_1 L_1|p_{in}|\alpha_2 L_2\rangle^{(L)}_{\nu_1 m_1} &= \langle \alpha_2 L_2|p_{in}|\alpha_1 L_1\rangle^{(L)}_{\nu_1 m_1}\\ &= \left\langle \left[\psi\begin{pmatrix}[\nu_1]\\ m_1,\ \alpha_1 L_1\end{pmatrix}\psi_l(n)\right]^L_M \middle| p_{in-1}p_{nn-1}p_{in-1} \middle| \left[\psi\begin{pmatrix}[\nu_1]\\ m_1,\alpha_2 L_2\end{pmatrix}\psi_l(n)\right]^L_M \right\rangle\\ &= \sum_{m_1'} \left[D^{[\nu_1]}_{m_1' m_1}(i,n-1)\right]^2 \langle \alpha_1 L_1|p_{nn-1}|\alpha_2 L_2\rangle^{(L)}_{\nu_1 m_1'}\ .\end{aligned} \tag{7-188}$$

From (7-182), (7-184)–(7-188) we obtain the eigenequation satisfied by the CFP.

$$\sum_{\alpha_2 L_2} \left[\langle \alpha_1 L_1|C'(n)|\alpha_2 L_2\rangle^L_{\nu_1} - \delta_{\alpha_1\alpha_2}\delta_{L_1L_2}(\nu-\nu_1)\right] C^{[\nu],\alpha L}_{[\nu_1]\alpha_2 L_2,[1]} = 0\ , \tag{7-189a}$$

where

$$\langle \alpha_1 L_1|C'(n)|\alpha_2 L_2\rangle^L_{\nu_1} = \sum_{i=1}^{n-1} \langle \alpha_1 L_1|p_{in}|\alpha_2 L_2\rangle^{(L)}_{\nu_1 m_1}\ . \tag{7-189b}$$

Notice that although each term on the right-hand side of (7-189b) depends on m_1, their sum is independent of m_1. Dividing (7-189b) by h_{ν_1}, summing over m_1 and using (7-188), we can show that

$$\langle \alpha_1 L_1|C'(n)|\alpha_2 L_2\rangle^L_{\nu_1} = \frac{n-1}{h_{\nu_1}} \sum_{m_1} \langle \alpha_1 L_1|p_{nn-1}|\alpha_2 L_2\rangle^{(L)}_{\nu_1 m_1}\ . \tag{7-189c}$$

Furthermore, since the above matrix elements of p_{nn-1} are independent of the component index m' of the irrep ν' of S_{n-2}, Eq. (7-189b) can be further simplified to

$$\langle \alpha_1 L_1|C'(n)|\alpha_2 L_2\rangle^L_{\nu_1} = \frac{n-1}{h_{\nu_1}} \sum_{\nu_1'} h_{\nu_1'} \langle \alpha_1 L_1|p_{nn-1}|\alpha_2 L_2\rangle^{(L)}_{\nu_1 \nu_1' m_1'}\ . \tag{7-189'}$$

Equation (7-189') provides a most effective way for computing the matrix of $C'(n)$.

If ν is a single root of the secular equation of (7-189a), the additional label α is redundant. If ν is a τ–fold root, then there are τ sets of eigensolutions $C^{[\nu]\alpha L}_{[\nu_1]\alpha_1 L_1,[1]}, \alpha = 1,2,\ldots,\tau$, which can be made orthogonal with respect to the index α.

From $[\nu]m = [\nu][\nu_1]m_1$ and (7-182) it is seen that different $[\nu_1]$ correspond to different components m of the irrep $[\nu]$. In the procedure described above, the eigenequation (7-189a) is solved individually for each $[\nu_1]$. As a consequence, the relative phases of the CFP $C^{[\nu]\alpha L}_{[\nu_1]\alpha_1 L_1,[1]}$ with respect to $C^{[\nu]\alpha L}_{[\overline{\nu}_1]\overline{\alpha}_1\overline{L}_1,[1]}$ are chosen randomly. What is more serious is that for the multiplicity–not–free cases, the multiplicity label α is also chosen randomly for each $[\nu_1]$. Therefore, the basis vectors $\psi\begin{pmatrix}[\nu]\\ m,\alpha L\end{pmatrix}$ and $\psi\begin{pmatrix}[\nu]\\ \overline{m},\alpha L\end{pmatrix}$ constructed from (7-182) in terms of the CFP $C^{[\nu]\alpha L}_{[\nu_1]\alpha_1 L_1,[1]}$ and $C^{[\nu]\alpha L}_{[\overline{\nu}_1]\overline{\alpha}_1\overline{L}_1,[1]}$, respectively, are in general not two partners of the same irrep $[\nu]$. These two shortcomings can be remedied by the following technique.

From (7-182), we have

$$D^{[\nu]}_{\overline{m}m}(n-1,n) = \left\langle \psi\left(\begin{matrix}[\nu]\\ \overline{m},\alpha L\end{matrix}\right)\middle| p_{n,n-1}\middle|\psi\left(\begin{matrix}[\nu]\\ m,\alpha L\end{matrix}\right)\right\rangle = \sum_{\alpha_1 L_1 \overline{\alpha}_1 \overline{L}_1 \alpha' L'} C^{[\nu]\alpha L}_{[\overline{\nu}_1]\overline{\alpha}_1\overline{L}_1,[1]}$$
$$\times C^{[\overline{\nu}_1]\overline{\alpha}_1\overline{L}_1}_{[\nu']\alpha' L',[1]} C^{[\nu]\alpha L}_{[\nu_1]\alpha_1 L_1,[1]} C^{[\nu_1]\alpha_1 L_1}_{[\nu']\alpha' L',[1]} \langle L'\overline{L}_1 L|p_{n-1,n}|L' L_1 L\rangle \ . \tag{7-189d}$$

As in our derivation of (4-195b) from (4-195a), we have from (7-189d)

$$C^{[\nu]\alpha L}_{[\overline{\nu}_1]\overline{\alpha}_1\overline{L}_1,[1]} = [D^{[\nu]}_{\overline{m}m}(n-1,n)]^{-1}$$
$$\times \sum_{\substack{\alpha_1 L_1\\ \alpha' L'}} \left[C^{[\overline{\nu}_1]\overline{\alpha}_1\overline{L}_1}_{[\nu']\alpha' L',[1]} C^{[\nu_1]\alpha_1 L_1}_{[\nu']\alpha' L',[1]} \langle L'\overline{L}_1 L|p_{n-1,n}|L' L_1 L\rangle\right] C^{[\nu]\alpha L}_{[\nu_1]\alpha_1 L_1,[1]} \ . \tag{7-189e}$$

Thus the correct procedure for computing the CFP is that for each possible $[\nu]$, we take the CFP $C^{[\nu]\alpha L}_{[\nu_1]\alpha_1 L_1,[1]}$ from the eigenvectors of (7-189a) only for a given $[\nu_1]$, while all the other CFP $C^{[\nu]\alpha L}_{[\overline{\nu}_1]\overline{\alpha}_1\overline{L}_1,[1]}$, for $\overline{\nu}_1 \neq \nu_1$, are to be calculated from (7-189e).

Equations (7-189) and (7-188c) provide a recursive way for calculating the CFP. This method is simpler than Jahn's (1951) method.

Example 7: Find the CFP for the $1p$ shell, $n = 3, [\nu_1] = [2]$ and $L = 1$. Since the irrep $[\nu_1] = [2]$ contains $L_1 = 0$ and 2, we now need to diagonalize $C'(3)$ in the basis $\varphi_1 = \left[|[2]S\rangle\psi(3)\right]^P$ and $\varphi_2 = \left[|[2]D\rangle\psi(3)\right]^P$. The CFP for $n = 2$ is equal to one, therefore from (7-187b) we have

$$\langle \alpha_1 L_1|p_{23}|\alpha_2 L_2\rangle^{(L)}_{[2]} = \langle PL_1 P|p_{23}|PL_2 P\rangle \ .$$

Using the table of Racah coefficients, we find the matrix $\langle PL_1 P|p_{23}|PL_2 P\rangle$ to be

PL_1 \ PL_2	PS	PD
PS	$\frac{1}{3}$	$\frac{\sqrt{5}}{3}$
PD	$\frac{\sqrt{5}}{3}$	$\frac{1}{6}$

The eigenvalue corresponding to $[\nu_1] = [2]$ is $\nu_1 = 1$. Using (7-189′) Eq. (7-189a) becomes

$$\begin{pmatrix} \frac{5}{3} - \nu & \frac{2\sqrt{5}}{3} \\ \frac{2\sqrt{5}}{3} & \frac{4}{3} - \nu \end{pmatrix} \begin{pmatrix} C^{[\nu]P}_{[2]S,[1]} \\ C^{[\nu]P}_{[2]D,[1]} \end{pmatrix} = 0 \ . \tag{7-190}$$

From (7-190) we find two single roots $\nu = 0$ and 3, corresponding to $[\nu] = [21]$ and $[3]$, respectively, and the CFP listed below

$[\nu]L$ \ $[\nu_1]L_1$	$[2]S$	$[2]D$
$[3]P$	$\frac{\sqrt{5}}{3}$	$\frac{2}{3}$
$[21]P$	$\frac{2}{3}$	$-\frac{\sqrt{5}}{3}$

In our example, (7-159b) takes the form

$$\left|\boxed{1\,2\,3}, PM\right\rangle = \left[\left(\tfrac{\sqrt{5}}{3}\left|\boxed{1\,2}, S\right\rangle + \tfrac{2}{3}\left|\boxed{1\,2}, D\right\rangle\right)\psi(3)\right]^P_M , \tag{7-191a}$$

$$\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}, PM\right\rangle = \left[\left(\tfrac{2}{3}\left|\boxed{1\,2}, S\right\rangle - \tfrac{\sqrt{5}}{3}\left|\boxed{1\,2}, D\right\rangle\right)\psi(3)\right]^P_M , \tag{7-191b}$$

or more succinctly

$$|[3]P\rangle = \left(\tfrac{\sqrt{5}}{3}|[2]S\rangle + \tfrac{2}{3}|[2]D\rangle\right)\psi(3) , \tag{7-191c}$$

$$|[21]P\rangle = \left(\tfrac{2}{3}|[2]S\rangle - \tfrac{\sqrt{5}}{3}|[2]D\rangle\right)\psi(3) . \tag{7-191d}$$

The rest of the CFP for $n = 3$ are trivial. They are either equal to one or zero, as determined by the angular momentum coupling rule. For example we have

$$|[21]D\rangle = C_1\left[|[2]D\rangle\psi_p(3)\right]^D + C_2\left[|[2]S\rangle\psi_p(3)\right]^D = \left[|[2]D\rangle\psi_p(3)\right]^D . \tag{7-192a}$$

$$|[21]D\rangle = \left[|[11]P\rangle\psi(3)\right]^D , \quad |[21]P\rangle = \left[|[11]P\rangle\psi(3)\right]^P . \tag{7-192b}$$

Example 8: Find the CFP for the $1p$ shell, $n = 4, [\nu_1] = [21], L = D$. From Table IC-4 in Bohr (1969), it is known that the irrep [21] contains $L_1 = P, D$. Thus we need to diagonalize $C'(4)$ in the basis (φ_1, φ_2), or (χ_1, χ_2):

$$\varphi_1 = \left[\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}, P\right\rangle\psi(4)\right]^D , \quad \varphi_2 = \left[\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}, D\right\rangle\psi(4)\right]^D ,$$

$$\chi_1 = \left[\left|\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}, P\right\rangle\psi(4)\right]^D , \quad \chi_2 = \left[\left|\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}, D\right\rangle\psi(4)\right]^D . \tag{7-193}$$

Using the CFP (7-191b), as well as (7-192), we expand the three-particle states in (7-193), giving

$$\begin{aligned} \varphi_1 &= \tfrac{2}{3}|SPD\rangle - \tfrac{\sqrt{5}}{3}|DPD\rangle , & \varphi_2 &= |DDD\rangle , \\ \chi_1 &= |PPD\rangle , & \chi_2 &= |PDD\rangle . \end{aligned} \tag{7-194}$$

From (7-187a), or Table 1 given by Jahn (1951), we find the matrix representatives of p_{34} in the bases (φ_1, φ_2) and (χ_1, χ_2):

$$\begin{aligned} (\langle\alpha_1 L_1|p_{34}|\alpha_2 L_2\rangle_{[21]m_1=1}) &= \mathcal{D}_1(34) = \begin{pmatrix} 1/2 & -\sqrt{3}/6 \\ -\sqrt{3}/6 & 5/6 \end{pmatrix} , \\ (\langle\alpha_1 L_1|p_{34}|\alpha_2 L_2\rangle_{[21]m_1=2}) &= \mathcal{D}_2(34) = \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} . \end{aligned} \tag{7-195}$$

From (7-189′) and (7-195), we obtain the matrix representative of $C'(4)$ in the basis (φ_1, φ_2) or (χ_1, χ_2),

$$\mathcal{D}_1(C'(4)) = \mathcal{D}_2(C'(4)) = \begin{pmatrix} 3/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix} . \tag{7-196}$$

By diagonalizing (7-196), the CFP $(p^3, p|\}p^4) = C^{[\nu]L}_{[\nu_1]L_1,[1]}$ are found to be

$[\nu]L$ \ $[\nu_1]L_1$	$[21]P$	$[21]D$
$[31]D$	$\sqrt{3}/2$	$1/2$
$[22]D$	$-1/2$	$\sqrt{3}/2$

that is

$$\left|\begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array}, DM\right\rangle = \left(\frac{\sqrt{3}}{2}\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}, P\right\rangle + \frac{1}{2}\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}, D\right\rangle\right)\psi(4)\ ,$$

$$\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\hline\end{array}, DM\right\rangle = \left(-\frac{1}{2}\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}, P\right\rangle + \frac{\sqrt{3}}{2}\left|\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}, D\right\rangle\right)\psi(4)\ , \tag{7-197a}$$

or more succinctly

$$\begin{aligned}|[31]D\rangle &= \left(\tfrac{\sqrt{3}}{2}|[21]P\rangle + \tfrac{1}{2}|[21]D\rangle\right)\psi(4)\ ,\\ |[22]D\rangle &= \left(-\tfrac{1}{2}|[21]P\rangle + \tfrac{\sqrt{3}}{2}|[21]D\rangle\right)\psi(4)\ .\end{aligned} \tag{7-197b}$$

The above technique can be easily extended to the calculation of any $SU_n \supset G$ CFP. Such as:

1. The $SU_3 \supset SU_2$ CFP. Corresponding to (7-182), we have

$$\psi\begin{pmatrix}[\nu]\\ m,\ IYI_Z\end{pmatrix} = \sum_{I_1Y_1} C^{[\nu]IY}_{[\nu_1]I_1Y_1,[1]}\left[\psi\begin{pmatrix}[\nu_1]\\ m_1,\ I_1Y_1\end{pmatrix}\psi(n)\right]^{I}_{I_Z}\ , \tag{7-198}$$

where $\nu_1 m_1 IY$ are fixed. The matrix elements in (7-187b) are replaced by the following

$$\begin{aligned}&\langle\alpha_1L_1|p_{n-1,n}|\alpha_2L_2\rangle^L \to \langle I_1Y_1|p_{n-1,n}|I_2Y_2\rangle^I\\ &= \sum_{I'Y'} C^{[\nu_1]I_1Y_1}_{[\nu']I'Y',[1]}C^{[\nu_1]I_2Y_2}_{[\nu']I'Y',[1]}\langle I'I_1I|p_{n-1,n}|I'I_2I\rangle\ .\end{aligned} \tag{7-199}$$

2. $SU_4 \supset SU_2 \times SU_2$ CFP

$$\psi\begin{pmatrix}[\nu]\\ m,\beta STM_SM_T\end{pmatrix} = \sum_{\beta_1S_1T_1} C^{[\nu]\beta ST}_{[\nu_1]\beta_1S_1T_1,[1]}\left[\psi\begin{pmatrix}[\nu_1]\\ m_1,\beta_1S_1T_1\end{pmatrix}\psi(n)\right]^{ST}_{M_SM_T}\ , \tag{7-200}$$

$$\begin{aligned}&\langle\alpha_1L_1|p_{n-1,n}|\alpha_2L_2\rangle \to \langle\beta_1S_1T_1|p_{n-1n}|\beta_2S_2T_2\rangle\\ &= \sum_{\beta'S'T'} C^{[\nu_1]\beta_1S_1T_1}_{[\nu']\beta'S'T',[1]}C^{[\nu_1]\beta_2S_2T_2}_{[\nu']\beta'S'T',[1]}\langle S'S_1S|p_{n-1n}|S'S_2S\rangle\langle T'T_1T|p_{n-1n}|T'T_2T\rangle\ .\end{aligned} \tag{7-201}$$

3. $SU_6 \supset SU_3 \times SU_2$ CFP.

$$\psi\begin{pmatrix}[\nu]\\ m,\beta(\lambda\mu)IYS\end{pmatrix} = \sum_{\beta_1(\lambda_1\mu_1)S_1} C^{[\nu]\beta(\lambda\mu)S}_{[\nu_1]\beta_1(\lambda_1\mu_1)S_1,[1]}\left[\psi\begin{pmatrix}[\nu_1]\\ m_1,\ \beta_1(\lambda_1\mu_1)I_1Y_1S_1\end{pmatrix}\psi(n)\right]^{(\lambda\mu)IYS}\ , \tag{7-202}$$

where we ignored the magnetic quantum numbers I_z, S_z, since the $SU_6 \supset SU_3 \times SU_2$ CFP are independent of these quantum numbers.

$$\langle \alpha_1 L_1 | p_{n-1,n} | \alpha_2 L_2 \rangle^L \to \langle \beta_1 (\lambda_1 \mu_1) S_1 | p_{n-1,n} | \beta_2 (\lambda_2 \mu_2) S_2 \rangle^{(\lambda\mu)S}$$

$$= \sum_{\beta'(\lambda'\mu')S'} C^{[\nu_1]\beta_1(\lambda_1\mu_1)S_1}_{[\nu']\beta'(\lambda'\mu')S',[1]} C^{[\nu_1]\beta_2(\lambda_2\mu_2)S_2}_{[\nu']\beta'(\lambda'\mu')S',[1]} \langle S' S_1 S | p_{n-1,n} | S' S_2 S \rangle$$
$$\times \langle (\lambda'\mu')(\lambda_1\mu_1)(\lambda\mu) | p_{n-1,n} | (\lambda'\mu')(\lambda_2\mu_2)(\lambda\mu) \rangle \ , \tag{7-203}$$

where

$$\langle (\lambda'\mu')(\lambda_1\mu_1)(\lambda\mu) | p_{n-1,n} | (\lambda'\mu')(\lambda_2\mu_2)(\lambda\mu) \rangle$$
$$= (-)^{\lambda'-\mu'+\lambda-\mu+\lambda_1-\mu_1+\lambda_2-\mu_2} U((10)(\lambda'\mu')(\lambda\mu)(10); (\lambda_1\mu_1)(\lambda_2\mu_2)) \ . \tag{7-204}$$

Many numerical tables, algebraic expressions and computer codes have been published for various kinds of CFP and ISF. We list some below.

1. $SU_3 \supset SO_3$. Tables of one–particle CFP are found in Jahn (1951). For two–particle CFP, see Elliott (1953). Tables of $SU_3 \supset SO_3$ ISF are given by Sun (1965). For algebraic expressions for the $SU_3 \supset SO_3$ ISF, consult Vergados (1968) and Horie (1964). Akiyama (1973) has given a computer code for $SU_3 \supset SO_3$ ISF.

2. $SU_3 \supset SU_2 \otimes U_1$ ISF. For numerical tables, see de Swart (1963). Algebraic expressions are found in Hecht (1965).

3. $SU_4 \supset SU_3 \otimes U_1$ ISF. Numerical tables are given by Rabl (1975), Haacke (1976).

4. $SU_n \supset SU_{n-1} \otimes U_1$ ISF with arbitrary m for for irreps involving only two columns. Algebraic formulas are derived by Li and Paldus (1990 [1]).

5. $SU_4 \supset SU_2 \times SU_2$. For one–particle CFP, see Jahn (1951). Two–particle CFP are given by Elliott (1953) and Harvey (1981). Algebraic expression may be found in Hecht (1969).

6. $SU_6 \supset SU_3 \times SU_2$ ISF. Numerical tables are collected in So (1979), Strottman (1979), Zhang (1977), Machacek (1976), Cook (1965).

7. $SU_6 \supset SU_3$ ISF. Numerical tables are given by Akiyama (1966). Algebraic expressions are compiled in Hecht (1965). Braunschweig (1978) gave computer code.

8. $SU_{15} \supset SU_3$ ISF. Computer code is given by Wu (1983).

9. $SU_{mn} \supset SU_m \times SU_n$ CFP for arbitrary m and n. Numerical tables are given in Chen, Wu & Gao (1991). Computer code for one–particle CFP is given by Novoselsky [1] (1988).

10. $SU_{m+n} \supset SU_m \otimes SU_n$ single particle CFP for arbitrary m and n. For numerical tables, see Chen, Chen & Gao (1984). Computer code for one–particle CFP is given by Novoselsky [1] (1988).

11. $SU_{2j+1} \supset Sp_{2j+1} \supset SO_3$ and $SU_{2l+1} \supset SO_{2l+1} \supset SO_3$ CFP Tables: a) for totally anti–symmetric and totally symmetric states respectively. See Bayman (1966). b) for arbitrary symmetries, see Novoselsky (1988).

12. The elementary reduced Wigner coefficients (analytic expression): Le Blanc (1987).

13. The $SO_5 \supset U_2$ ISF analytic expression: Hecht (1989).

14. The CFP's for bosons (Han 1995) and fermions (Sun 1993, Wang 1995).

7.14. The $S_f \supset S_{f_1} \otimes S_{f_2} \otimes S_{f_3}$ Irreducible Basis and SU_n Racah Coefficients*

This section is similar to Sec. 7.10. The difference is that the unitary and permutation groups interchange their roles.

We begin with the construction of the $S_f \supset S_{f_1} \otimes S_{f_2} \otimes S_{f_3}$ irreducible basis, with $f = f_1 + f_2 + f_3, S_{f_i} \equiv S_{f_i}(\omega_i^0)$, the definition of (ω_1^0) and (ω_2^0) being the same as in the previous section, $(\omega_3^0) = (f_1 + f_2 + 1, \ldots, f_1 + f_2 + f_3)$. There are two ways of constructing such a basis.

1. The $S_f \supset (S_{f_1+f_2} \supset S_{f_1} \otimes S_{f_2}) \otimes S_{f_3}$ irreducible basis. According to (7-102b), it can be expressed as

$$\left| \begin{matrix} [\nu] \\ w, \end{matrix} \begin{pmatrix} [\nu_{12}] & [\nu_3] \\ \nu_1 m_1 \nu_2 m_2 & , m_3 \end{pmatrix} \right\rangle^{\tau_{12}\tau} = \sum_{w_1 w_2 w_3 w_{12}} C^{[\nu_{12}]\tau_{12}, w_{12}}_{\nu_1 w_1, \nu_2 w_2} C^{[\nu]\tau, w}_{\nu_{12} w_{12}, \nu_3 w_3} \left| \begin{matrix} [\nu_1] \\ m_1\omega_1^0, \ w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ m_2\omega_2^0, \ w_2 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_3] \\ m_3\omega_3^0, \ w_3 \end{matrix} \right\rangle . \tag{7-205a}$$

It is an irreducible basis $[\nu]w$ of SU_n and Yamanouchi basis $[\nu_i]m_i$ of S_{f_i}, and it belongs to the irrep $[\nu]$ and $[\nu_{12}]$ of S_f and $S_{f_1+f_2}$, respectively.

2. The $S_f \supset S_{f_1} \otimes (S_{f_2+f_3} \supset S_{f_2} \otimes S_{f_3})$ irreducible basis. In this case we have

$$\left| \begin{matrix} [\nu] \\ w, \end{matrix} \begin{pmatrix} [\nu_1] & [\nu_{23}] \\ m_1, & \nu_2 m_2 \nu_3 m_3 \end{pmatrix} \right\rangle^{\tau_{23}\tau'} = \sum_{w_1 w_2 w_3 w_{23}} C^{[\nu_{23}]\tau_{23}, w_{23}}_{\nu_2 w_2, \nu_3 w_3} C^{[\nu]\tau', w}_{\nu_1 w_1, \nu_{23} w_{23}} \left| \begin{matrix} [\nu_1] \\ m_1\omega_1^0, \ w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ m_2\omega_2^0, \ w_2 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_3] \\ m_3\omega_3^0, \ w_3 \end{matrix} \right\rangle . \tag{7-205b}$$

The bases in (7-205a) and (7-205b) are related by a unitarity transformation:

$$\left| \begin{matrix} [\nu] \\ w, \end{matrix} \begin{pmatrix} [\nu_{12}] & [\nu_3] \\ \nu_1 m_1 \nu_2 m_2, & m_3 \end{pmatrix} \right\rangle^{\tau_{12}\tau} = \sum_{\nu_{23}\tau_{23}\tau'} U(\nu_1\nu_2\nu\nu_3, \nu_{12}\nu_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} \left| \begin{matrix} [\nu] \\ w, \end{matrix} \begin{pmatrix} [\nu_1] & [\nu_{23}] \\ m_1, & \nu_2 m_2 \nu_3 m_3 \end{pmatrix} \right\rangle^{\tau_{23}\tau'} , \tag{7-206a}$$

where the U are the *Racah coefficients* of SU_n , the values of which are independent of w, m_1, m_2 and m_3. If we are only interested in the unitary group SU_2, (7-206a) can be cast into a form familiar in angular momentum theory

$$|([\nu_1][\nu_2])[\nu_{12}], [\nu_3] : [\nu]w\rangle^{\tau_{12},\tau} = \sum_{\nu_{23}\tau_{23}\tau'} U(\nu_1\nu_2\nu\nu_3, \nu_{12}\nu_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} |[\nu_1]([\nu_2][\nu_3])[\nu_{23}]; \ [\nu]w\rangle^{\tau_{23}\tau'} . \tag{7-206b}$$

From (7-204) and (7-205) we obtain

$$U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} = \sum_{\text{fix } w} C^{[\nu_{12}]\tau_{12}, w_{12}}_{\nu_1 w_1, \nu_2 w_2} C^{[\nu]\tau, w}_{\nu_{12} w_{12}, \nu_3 w_3} C^{[\nu_{23}]\tau_{23}, w_{23}}_{\nu_2 w_2, \nu_3 w_3} C^{[\nu]\tau', w}_{\nu_1 w_1, \nu_{23} w_{23}} . \tag{7-207}$$

The formula (7-124) to (7-130) for the Racah coefficients of permutation groups are also valid for the unitary group SU_n, if we make the following index substitutions: $m \to w, m_i \to w_i, \tau \to \beta$, and interpret the dimensions such as h_ν and h_{ν_κ} as dimensions of irreps of SU_n.

The CG coefficients of SU_n depend on the choice of the classification scheme for the irreducible basis, while the Racah coefficients do not. The latter only depend on the irreps.

Example 1: The Racah coefficients of SU_3.

a. In the $SU_3 \supset SU_2 \times U_1$ irreducible basis, by substituting (7-148) into (7-207) we have

$$U(\mu_1\mu_2\mu\mu_3, \mu_{12}\mu_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} = \sum_{\overline{w}_1\overline{w}_2\overline{w}_3\overline{w}_{12}\overline{w}_{23}} U(I_1I_2II_3; I_{12}I_{23})\{CCCC\} , \tag{7-208a}$$

where

$$\{CCCC\} = C^{[\mu_{12}],\tau_{12}\overline{w}_{12}}_{\mu_1\overline{w}_1,\mu_2\overline{w}_2} C^{[\mu]\tau,\overline{w}}_{\mu_{12}\overline{w}_{12},\mu_3\overline{w}_3} C^{[\mu]\tau',\overline{w}}_{\mu_1\overline{w}_1,\mu_{23}\overline{w}_{23}} C^{[\mu_{23}]\tau_{23},\overline{w}_{23}}_{\mu_2\overline{w}_2,\mu_3\overline{w}_3} , \tag{7-208b}$$

with $\overline{w} = IY, \overline{w}_i = I_iY_i$.

b. In the $SU_3 \supset SO_3 \supset SO_2$ basis, the CG coefficients can be factorized as

$$C^{[\mu]\tau,\kappa LM}_{[\mu_1]\kappa_1L_1M_1,[\mu_2]\kappa_2L_2M_2} = C^{[\mu]\tau,\kappa L}_{[\mu_1]\kappa_1L_1,[\mu_2]\kappa_2L_2} C^{LM}_{L_1M_1,L_2M_2} , \tag{7-209}$$

where the index κ is the multiplicity label on the reduction of the irrep $[\mu]$ of SU_3 into the irreps (L) of SO_3. The Racah coefficient of SU_3 is now expressed as

$$U(\mu_1\mu_2\mu\mu_3; \mu_{12}\mu_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} = \sum_{\overline{w}_1\overline{w}_2\overline{w}_3\overline{w}_{12}\overline{w}_{23}} U(L_1L_2LL_3; L_{12}L_{23})\{CCCC\} , \tag{7-210}$$

where $\{CCCC\}$ is still given by (7-208b) with the understanding that now $\overline{w} = \kappa L$ and $\overline{w}_i = \kappa_i L_i$.

If all the multiplicity labels $\tau_{12}, \tau_{23}, \tau$ and τ' are redundant, then the Racah coefficients evaluated from (7-208a) and (7-210) must be equal to within a phase factor. For the case when any of the multiplicity labels have more than one possible value, the Racah coefficients of (7-208a) and (7-210) may differ by a linear transformation.

Example 2: The Racah coefficients of SU_4. We choose the $SU_4 \supset SU_2 \times SU_2$ irreducible basis. Substituting (7-155) into (7-207), we have

$$\begin{aligned} &U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} \\ &\quad = \sum_{\overline{w}_1\overline{w}_2\overline{w}_3\overline{w}_4} U(S_1S_2SS_3; S_{12}S_{23})U(T_1T_2TT_3; T_{12}T_{23})\{CCCC\} , \end{aligned} \tag{7-211a}$$

where $\{CCCC\}$ is still given by (7-208b) with $\overline{w} = \beta ST, \overline{w}_i = \beta_i S_i T_i$. As in (7-130) we have

$$\begin{aligned} &\sum_{\tau'} U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} C^{[\nu]\tau,\overline{w}}_{\nu_1\overline{w}_1,\nu_{23}\overline{w}_{23}} \\ &\quad = \sum_{\overline{w}_2\overline{w}_3\overline{w}_{12}} U(S_1S_2SS_3; S_{12}S_{23})U(T_1T_2TT_3; T_{12}T_{23}) \\ &\quad \times C^{[\nu_{12}]\tau_{12},\overline{w}_{12}}_{\nu_1\overline{w}_1,\nu_2\overline{w}_2} C^{[\nu]\tau,\overline{w}}_{\nu_{12}\overline{w}_{12},\nu_3\overline{w}_3} C^{[\nu_{23}]\tau_{23},\overline{w}_{23}}_{\nu_2\overline{w}_2,\nu_3\overline{w}_3} . \end{aligned} \tag{7-211b}$$

Draayer (1973), and Sun (1980) discussed the Racah coefficients of SU_3; Hecht (1969), the Racah coefficients of SU_4; Kaplan (1961) and Le Blanc (1987), and Li & Paldus (1990a) the Racah coefficients of SU_n; Derome (1965, 1966), the Racah algebra for an arbitrary group.

7.15. The $\mathbf{S}_f \supset \mathbf{S}_{f_1} \otimes \mathbf{S}_{f_2} \otimes \mathbf{S}_{f_3} \otimes \mathbf{S}_{f_4}$ Irreducible Basis and the 9ν–Coefficients of $\mathbf{SU}_n$*

7.15.1. The 9ν–coefficients of SU_n

Let us introduce the following symbols for particle numbers:

$$\begin{aligned} &f_{12} = f_1 + f_2 , \quad f_{34} = f_3 + f_4 , \quad f_{13} = f_1 + f_3 , \quad f_{24} = f_2 + f_4 , \\ &f_{123} = f_{12} + f_3 , \quad f = f_{12} + f_{34} = f_{13} + f_{24} . \end{aligned} \tag{7-212a}$$

Let the four normal order sequences be

$$(\omega_1^0) = (1, 2, \ldots, f_1)\ , \qquad (\omega_2^0) = (f_1 + 1, \ldots, f_{12})\ ,$$
$$(\omega_3^0) = (f_{12} + 1, \ldots, f_{123})\ , \quad (\omega_4^0) = (f_{123} + 1, \ldots, f)\ . \tag{7-212b}$$

The permutation groups $S_{f_i}(\omega_i^0)$ are designated S_{f_i}.

We can use the following two ways to obtain the $S_f \supset S_{f_1} \otimes S_{f_2} \otimes S_{f_3} \otimes S_{f_4}$ irreducible basis.

1. The $S_f \supset (S_{f_{12}} \supset S_{f_1} \otimes S_{f_2}) \otimes (S_{f_{34}} \supset S_{f_3} \otimes S_{f_4})$ irreducible basis:

$$\left| \begin{matrix} [\nu] \\ w, \end{matrix} \begin{pmatrix} [\nu_{12}] & [\nu_{34}] \\ \nu_1 m_1 \nu_2 m_2, & \nu_3 m_3 \nu_4 m_4 \end{pmatrix} \right\rangle^{\tau_{12}\tau_{34}\tau} = \sum_{\substack{w_1 w_2 w_3 w_4 \\ w_{12} w_{34}}} C^{[\nu_{12}]\tau_{12}, w_{12}}_{\nu_1 w_1, \nu_2 w_2} C^{[\nu_{34}]\tau_{34}, w_{34}}_{\nu_3 w_3, \nu_4 w_4}$$
$$\times C^{[\nu]\tau, W}_{\nu_{12} w_{12}, \nu_{34} w_{34}} \left| \begin{matrix} [\nu_1] \\ m_1 \omega_1^0, w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ m_2 \omega_2^0, w_2 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_3] \\ m_3 \omega_3^0, w_3 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_4] \\ m_4 \omega_4^0, w_4 \end{matrix} \right\rangle . \tag{7-213a}$$

The left-hand side of (7-213a) is the irreducible basis $[\nu]w$ and $[\nu_i]m_i$ of SU_n and S_{f_i}, respectively, and it also belongs to the irrep $[\nu], [\nu_{12}]$ and $[\nu_{34}]$ of $S_f, S_{f_{12}}$ and $S_{f_{34}}$, respectively.

2. The $S_f \supset (S_{f_{13}} \supset S_{f_1} \otimes S_{f_3}) \otimes (S_{f_{24}} \supset S_{f_2} \otimes S_{f_4})$ irreducible basis

$$\left| \begin{matrix} [\nu] \\ w, \end{matrix} \begin{pmatrix} [\nu_{13}] & [\nu_{24}] \\ \nu_1 m_1 \nu_3 m_3, & \nu_2 m_2 \nu_4 m_4 \end{pmatrix} \right\rangle\!\!\rangle^{\tau_{13}\tau_{24}\tau'} = \sum_{\substack{w_1 w_2 w_3 w_4 \\ w_{13} w_{24}}} C^{[\nu_{13}]\tau_{13}, w_{13}}_{\nu_1 w_1, \nu_3 w_3} C^{[\nu_{24}]\tau_{24}, w_{24}}_{\nu_2 w_2, \nu_4 w_4}$$
$$\times C^{[\nu]\tau', w}_{\nu_{13} w_{13}, \nu_{24} w_{24}} \left| \begin{matrix} [\nu_1] \\ m_1 \omega_1^0, w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ m_2 \omega_2^0, w_2 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_3] \\ m_3 \omega_3^0, w_3 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_4] \\ m_4 \omega_4^0, w_4 \end{matrix} \right\rangle , \tag{7-213b}$$

where we use the symbol $|\ \rangle\!\rangle$ to distinguish (7-213b) from (7-218) to be given below. The bases (7-213a) and (7-213b) differ by a unitary transformation

$$\left| \begin{matrix} [\nu] \\ w, \end{matrix} \begin{pmatrix} [\nu_{12}] & [\nu_{34}] \\ \nu_1 m_1 \nu_2 m_2, & \nu_3 m_3 \nu_4 m_4 \end{pmatrix} \right\rangle^{\tau_{12}\tau_{34}\tau}$$
$$= \sum_{\substack{\nu_{13}\nu_{24} \\ \tau_{13}\tau_{24}\tau'}} \begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ \nu_3 & \nu_4 & \nu_{34} \\ \nu_{13} & \nu_{24} & \nu \end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} \left| \begin{matrix} [\nu] \\ w, \end{matrix} \begin{pmatrix} [\nu_{13}] & [\nu_{24}] \\ \nu_1 m_1 \nu_3 m_3, & \nu_2 m_2 \nu_4 m_4 \end{pmatrix} \right\rangle\!\!\rangle^{\tau_{13}\tau_{24}\tau'} . \tag{7-214a}$$

The first factor on the left-hand side of (7-214a) is a 9ν *coefficient* of SU_n , analogous of the $9j$ coefficients of SU_2, which is independent of the indices $w, m_1, \ldots, m_4$. Therefore if we focus our attention solely on the unitary group, (7-214a) can be rewritten as

$$|(\nu_1\nu_2)\nu_{12}, (\nu_3\nu_4)\nu_{34} : [\nu]w\rangle^{\tau_{12}\tau_{34}\tau}$$
$$= \sum_{\substack{\nu_{13}\nu_{24}\tau' \\ \tau_{13}\tau_{24}}} \begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ \nu_3 & \nu_4 & \nu_{34} \\ \nu_{13} & \nu_{24} & \nu \end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} |(\nu_1\nu_3)\nu_{13}, (\nu_2\nu_4)\nu_{24} : [\nu]w\rangle^{\tau_{13}\tau_{24}\tau'} . \tag{7-214b}$$

As with (7-136), the 9ν coefficients of SU_n can be expressed in terms of the 9μ coefficients of a subgroup G_s of SU_n and the $SU_n \supset G_s$ ISF. For example, in the $SU_4 \supset SU_2 \times SU_2$ classification,

the 9ν coefficients of SU_4 can be expressed as

$$\begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ \nu_3 & \nu_4 & \nu_{34} \\ \nu_{13} & \nu_{24} & \nu \end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} = \sum_{\text{fix}\,\overline{w}} \begin{pmatrix} S_1 & S_2 & S_{12} \\ S_3 & S_4 & S_{34} \\ S_{13} & S_{24} & S \end{pmatrix} \begin{pmatrix} T_1 & T_2 & T_{12} \\ T_3 & T_4 & T_{34} \\ T_{13} & T_{24} & T \end{pmatrix}$$

$$\times C^{[\nu_{12}]\tau_{12},\overline{w}_{12}}_{\nu_1\overline{w}_1,\nu_2\overline{w}_2} C^{[\nu_{34}]\tau_{34},\overline{w}_{34}}_{\nu_3\overline{w}_3,\nu_4\overline{w}_4} C^{[\nu]\tau,\overline{w}}_{\nu_{12}\overline{w}_{12},\nu_{34}\overline{w}_{34}} C^{[\nu_{13}]\tau_{13},\overline{w}_{13}}_{\nu_1\overline{w}_1,\nu_3\overline{w}_3} C^{[\nu_{24}]\tau_{24},\overline{w}_{24}}_{\nu_2\overline{w}_2,\nu_4\overline{w}_4} C^{[\nu]\tau',\overline{w}}_{\nu_{13}\overline{w}_{13},\nu_{24}\overline{w}_{24}} , \quad (7\text{-}215)$$

where $\overline{w} = \beta S T$, and $\overline{w}_i = \beta_i S_i T_i$.

Equations (7-134)-(7-138) are also applicable to the group SU_n after the index substitutions $m \to w, m_i \to w_i$, and the re–interpretation of the h's as the dimensions of the irreps of SU_n.

7.15.2. Evaluation of the Racah coefficients and 9ν coefficients of SU_n

For high order unitary groups, due to the difficulty in the calculation of the CG coefficients, it is not feasible to evaluate the Racah or 9ν coefficients by means of (7-134). This section and Sec. 9.4 will give two other methods for calculating these coefficients.

Let us first consider the 9ν coefficients. Define the permutation operator

$$P = \begin{pmatrix} \omega_2^0 & \omega_3^0 \\ \omega_3^0 & \omega_2^0 \end{pmatrix} = \begin{pmatrix} f_1+1, & f_1+2, & \ldots, & f_{12}, & f_{12}+1, \ldots, & f_{123} \\ f_{12}+1, & f_{12}+2, \ldots, & f_{123}, & f_1+1, & \ldots, & f_{12} \end{pmatrix} . \quad (7\text{-}216)$$

As an example, for $f_1 = 2, f_2 = 3, f_3 = 4, f_{12} = 5, f_{13} = 6, f_{123} = 9$, we have

$$P = \begin{pmatrix} 3\,4\,5\,6\,7\,8\,9 \\ 6\,7\,8\,9\,3\,4\,5 \end{pmatrix} = (3695847) .$$

Let $S'_{f_3} = S_{f_3}(\omega'_3), S'_{f_2} = S_{f_2}(\omega'_2)$, where

$$(\omega'_3) = (f_1+1, f_1+2, \ldots, f_{13}), \quad (\omega'_2) = (f_{13}+1, \ldots, f_{123}) . \quad (7\text{-}217)$$

The $S_f \supset (S'_{f_{13}} \supset (S_{f_1} \otimes S'_{f_3})) \otimes (S'_{f_{24}} \supset (S'_{f_2} \otimes S_{f_4}))$ irreducible basis can be expressed as

$$\left| \begin{matrix} [\nu] \\ w, \end{matrix} \begin{pmatrix} [\nu_{13}] & [\nu_{24}] \\ \nu_1 m_1 \nu_3 m_3, & \nu_2 m_2 \nu_4 m_4 \end{pmatrix} \right\rangle^{\tau_{13}\tau_{24}\tau'} = \sum_{\substack{w_1 w_2 w_3 w_4 \\ w_{13} w_{24}}} C^{[\nu_{13}]\tau_{13},w_{13}}_{\nu_1 w_1,\nu_3 w_3} C^{[\nu_{24}]\tau_{24},w_{24}}_{\nu_2 w_2,\nu_4 w_4} C^{[\nu]\tau',w}_{\nu_{13} w_{13},\nu_{24} w_{24}}$$

$$\times \left| \begin{matrix} [\nu_1] \\ m_1\omega_1^0, w_1 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_2] \\ m_2\omega'_2, w_2 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_3] \\ m_3\omega'_3, w_3 \end{matrix} \right\rangle \left| \begin{matrix} [\nu_4] \\ m_4\omega_4^0, w_4 \end{matrix} \right\rangle . \quad (7\text{-}218)$$

Notice that (7-218) and (7-213) have exactly the same quantum numbers and they differ only in the indices of the particles belonging to the irrep $[\nu_2]$ and $[\nu_3]$. Using (7-214a) and (7-218), the 9ν coefficients can be expressed as (Kramer 1967),

$$\begin{pmatrix} \nu_1 & \nu_2 & \nu_{12} \\ \nu_3 & \nu_4 & \nu_{34} \\ \nu_{13} & \nu_{24} & \nu \end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} = \left\langle [\nu] \begin{pmatrix} [\nu_{12}] & [\nu_{34}] \\ \nu_1 m_1 \nu_2 m_2, & \nu_3 m_3 \nu_4 m_4 \end{pmatrix}^{\tau_{12}\tau_{34}\tau} \right.$$

$$\times \left| \begin{pmatrix} \omega_2^0 & \omega_3^0 \\ \omega_3^0 & \omega_2^0 \end{pmatrix} \right| \left. [\nu] \begin{pmatrix} [\nu_{13}] & [\nu_{24}] \\ \nu_1 m_1 \nu_3 m_3, & \nu_2 m_2 \nu_4 m_4 \end{pmatrix}^{\tau_{13}\tau_{24}\tau'} \right\rangle , \quad (7\text{-}219)$$

where we suppressed the index w. Using the SDC in (4-168a), the non-standard bases of the

permutation groups in (7-219) can be expanded in terms of the standard bases, as for instance

$$\left|[\nu]\begin{pmatrix}[\nu_{12}] & [\nu_{34}]\\ \nu_1 m_1 \nu_2 m_2, & \nu_3 m_3 \nu_4 m_4\end{pmatrix}\right\rangle^{\tau_{12}\tau_{34}\tau} = \sum_{m m_{12} m_{34}} \left|\begin{matrix}[\nu]\\ m\end{matrix}\right\rangle \left\langle\begin{matrix}[\nu]\\ m\end{matrix}\right| [\nu]\begin{matrix}\tau[\nu_{12}][\nu_{34}]\\ m_{12}\ m_{34}\end{matrix}\Big\rangle$$
$$\times \left\langle\begin{matrix}[\nu_{12}]\\ m_{12}\end{matrix}\right| [\nu_{12}],\ \begin{matrix}\tau_{12}[\nu_1][\nu_2]\\ m_1\ m_2\end{matrix}\Big\rangle \left\langle\begin{matrix}[\nu_{34}]\\ m_{34}\end{matrix}\right| [\nu_{34}],\ \begin{matrix}\tau_{34}[\nu_3][\nu_4]\\ m_3\ m_4\end{matrix}\Big\rangle . \tag{7-220}$$

Interchanging $2 \leftrightarrow 3$, we find a similar expression for (7-218). Combining (7-219) and (7-220) we obtain

$$\begin{pmatrix}\nu_1 & \nu_2 & \nu_{12}\\ \nu_3 & \nu_4 & \nu_{34}\\ \nu_{13} & \nu_{24} & \nu\end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} = \sum_{\substack{m_{12} m_{34} m\\ m_{13} m_{24} m'}} D^{[\nu]}_{m m'}(P) \left\langle\begin{matrix}[\nu]\\ m\end{matrix}\right| [\nu],\ \begin{matrix}\tau[\nu_{12}][\nu_{34}]\\ m_{12}\ m_{34}\end{matrix}\Big\rangle$$
$$\times \left\langle\begin{matrix}[\nu_{12}]\\ m_{12}\end{matrix}\right| [\nu_{12}],\ \begin{matrix}\tau_{12}[\nu_1][\nu_2]\\ m_1\ m_2\end{matrix}\Big\rangle \left\langle\begin{matrix}[\nu_{34}]\\ m_{34}\end{matrix}\right| [\nu_{34}],\ \begin{matrix}\tau_{34}[\nu_3][\nu_4]\\ m_3\ m_4\end{matrix}\Big\rangle \left\langle\begin{matrix}[\nu]\\ m'\end{matrix}\right| [\nu],\ \begin{matrix}\tau'[\nu_{13}][\nu_{24}]\\ m_{13}\ m_{24}\end{matrix}\Big\rangle$$
$$\times \left\langle\begin{matrix}[\nu_{13}]\\ m_{13}\end{matrix}\right| [\nu_{13}],\ \begin{matrix}\tau_{13}[\nu_1][\nu_3]\\ m_1\ m_3\end{matrix}\Big\rangle \left\langle\begin{matrix}[\nu_{24}]\\ m_{24}\end{matrix}\right| [\nu_{24}],\ \begin{matrix}\tau_{24}[\nu_2][\nu_4]\\ m_2\ m_4\end{matrix}\Big\rangle , \tag{7-221a}$$

where the sum is carried out under fixed m_1, m_2, m_3 and m_4.

By letting $f_3 = 0, [\nu_3] = [0]$, and $P = e$ (identity), from (7-137) and (7-221a) we obtain an expression for the SU_n Racah coefficients (Kramer 1968):

$$U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} = \sum_{m_{12} m_{23} m} \left\langle\begin{matrix}[\nu]\\ m\end{matrix}\right| [\nu],\ \begin{matrix}\tau[\nu_{12}][\nu_3]\\ m_{12}\ m_3\end{matrix}\Big\rangle \left\langle\begin{matrix}[\nu_{12}]\\ m_{12}\end{matrix}\right| [\nu_{12}],\ \begin{matrix}\tau_{12}[\nu_1][\nu_2]\\ m_1\ m_2\end{matrix}\Big\rangle$$
$$\times \left\langle\begin{matrix}[\nu]\\ m\end{matrix}\right| [\nu],\ \begin{matrix}\tau'[\nu_1][\nu_{23}]\\ m_1\ m_{23}\end{matrix}\Big\rangle \left\langle\begin{matrix}[\nu_{23}]\\ m_{23}\end{matrix}\right| [\nu_{23}],\ \begin{matrix}\tau_{23}[\nu_2][\nu_3]\\ m_2 m_3\end{matrix}\Big\rangle , \tag{7-221b}$$

where the sum is carried out with m_1, m_2 and m_3 fixed.

Since the SDC of the permutation groups do not depend on n, we reach a significant conclusion that the *Racah coefficients as well as the 9ν coefficients of the group SU_n do not depend on n explicitly.* In other words, they only depend on the partition labels. Therefore we can tabulate the Racah coefficients and 9ν coefficients of the group SU_n for arbitrary n instead of each table referring to only one particular n.

The SDC of permutation groups can be easily calculated by the EFM. Consequently we can use (7-221a) and (7-221b) to calculate the Racah coefficients and 9ν coefficients of the group SU_n for arbitrary n. The SU_n Racah coefficients have been calculated in this way and tabulated in Chen, Wang, Lü & Wu (1987).

Utilizing the symmetries (4-180) and (4-67) of the SDC, and the irreducible matrix elements of S_f, we get from (7-221) the following two symmetries:

$$\begin{pmatrix}\tilde{\nu}_1 & \tilde{\nu}_2 & \tilde{\nu}_{12}\\ \tilde{\nu}_3 & \tilde{\nu}_4 & \tilde{\nu}_{34}\\ \tilde{\nu}_{13} & \tilde{\nu}_{24} & \tilde{\nu}\end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} = \varepsilon \cdot \begin{pmatrix}\nu_1 & \nu_2 & \nu_{12}\\ \nu_3 & \nu_4 & \nu_{34}\\ \nu_{13} & \nu_{24} & \nu\end{pmatrix}^{\tau_{12}\tau_{34}\tau}_{\tau_{13}\tau_{24}\tau'} , \tag{7-222a}$$

$$U(\tilde{\nu}_1\tilde{\nu}_2\tilde{\nu}\tilde{\nu}_3, \tilde{\nu}_{12}\tilde{\nu}_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} = \varepsilon U(\nu_1\nu_2\nu\nu_3; \nu_{12}\nu_{23})^{\tau_{12}\tau}_{\tau_{23}\tau'} \tag{7-222b}$$

where $\varepsilon = \pm 1$ is a phase depending on our phase choices.

Hecht (1975) studied the 9ν coefficients of SU_3 and SU_4; Kukulin (1967), the 9ν coefficients of SU_4; and Kramer (1969), the 9ν coefficients of SU_n.

7.16. $SU_{mn} \supset SU_m \times SU_n$ CFP*

7.16.1. $SU_{mn} \supset SU_m \times SU_n$ CFP and $S_{f_1+f_2} \supset S_{f_1} \otimes S_{f_2}$ ISF

In Sec. 7.12 we introduced a method for calculating the $SU_{mn} \supset SU_m \times SU_n$ CFP, where the Racah coefficients of SU_m and SU_n must be known beforehand. However, for $m > 3$, no tables of SU_m Racah coefficients are available. Therefore we have to seek after new methods.

As with (4-197), we introduce the following symbols to denote the irreps of the three unitary groups and nine permutation groups:

$$\begin{pmatrix} \sigma' & \mu' & \nu'_{\beta'} \\ \sigma'' & \mu'' & \nu''_{\beta''} \\ \sigma_\theta & \mu_\varphi & \nu_{\tau,\beta} \end{pmatrix}, \quad \begin{pmatrix} SU_m & SU_n & SU_{mn} \\ SU_m & SU_n & SU_{mn} \\ SU_m & SU_n & SU_{mn} \end{pmatrix}, \quad \begin{pmatrix} S_{f_1}(x) & S_{f_1}(\xi) & S_{f_1}(q) \\ S_{f_2}(x) & S_{f_2}(\xi) & S_{f_2}(q) \\ S_f(x) & S_f(\xi) & S_f(q) \end{pmatrix} \tag{7-223}$$

By making the following index substitutions,

$$\Lambda \to \sigma\mu\,, \quad m \to w_1 w_2\,, \quad \theta \to \theta\varphi\,, \quad 1 \to', 2 \to''\,,$$

we get the following equations from (3-300), (3-301) and (3-307),

$$\left| \begin{matrix} [\nu]\tau \\ \beta\sigma w_1 \mu w_2 \end{matrix} \right\rangle = \sum_{\substack{\beta'\sigma'\mu'\theta \\ \beta''\sigma''\mu''\varphi}} C^{[\nu]_\tau,\beta[\sigma]_\theta[\mu]_\varphi}_{\nu'\beta'\sigma'\mu',\nu''\beta''\sigma''\mu''} \left[\left| \begin{matrix} [\nu'] \\ \beta'\sigma'\mu' \end{matrix} \right\rangle \left| \begin{matrix} [\nu''] \\ \beta''\sigma''\mu'' \end{matrix} \right\rangle \right]^{[\sigma]_\theta[\mu]_\varphi}_{w_1 w_2} . \tag{7-224a}$$

$$\begin{aligned} &\left[\left| \begin{matrix} [\nu'] \\ \beta'\sigma'\mu' \end{matrix} \right\rangle \left| \begin{matrix} [\nu''] \\ \beta''\sigma''\mu'' \end{matrix} \right\rangle \right]^{[\sigma]_\theta[\mu]_\varphi}_{w_1 w_2} \\ &= \sum_{w'_1 w'_2 w''_1 w''_2} C^{[\sigma]_\theta,w_1}_{\sigma' w'_1,\sigma'' w''_1} C^{[\mu]_\varphi,w_2}_{\mu' w'_2,\mu'' w''_2} \left| \begin{matrix} [\nu'] \\ \beta'\sigma' w'_1 \mu' w'_2 \end{matrix} \right\rangle \left| \begin{matrix} [\nu''] \\ \beta''\sigma'' w''_1 \mu'' w''_2 \end{matrix} \right\rangle . \end{aligned} \tag{7-225}$$

$$\left[\left| \begin{matrix} [\nu'] \\ \beta'\sigma'\mu' \end{matrix} \right\rangle \left| \begin{matrix} [\nu''] \\ \beta''\sigma''\mu'' \end{matrix} \right\rangle \right]^{[\sigma]_\theta[\mu]_\varphi}_{w_1 w_2} = \sum_{\nu\tau\beta} C^{[\nu]_\tau,\beta[\sigma]_\theta[\mu]_\varphi}_{\nu'\beta'\sigma'\mu',\nu''\beta''\sigma''\mu''} \left| \begin{matrix} [\nu]\tau \\ \beta\sigma w_1 \mu w_2 \end{matrix} \right\rangle . \tag{7-226}$$

Equation (7-226) is the inverse of (7-224a). The first factor on the right-hand side of (7-224a) is the $SU_{mn} \supset SU_m \times SU_n$ ISF and is independent of w_1 and w_2. Therefore (7-224a) can be written succinctly as

$$\left| \begin{matrix} [\nu]\tau \\ \beta\sigma\mu \end{matrix} \right\rangle = \sum_{\substack{\beta'\sigma'\mu'\theta \\ \beta''\sigma''\mu''\varphi}} C^{[\nu]_\tau,\beta[\sigma]\theta[\mu]\varphi}_{\nu'\beta'\sigma'\mu',\nu''\beta''\sigma''\mu''} \left[\left| \begin{matrix} [\nu'] \\ \beta'\sigma'\mu' \end{matrix} \right\rangle \left| \begin{matrix} [\nu''] \\ \beta''\sigma''\mu'' \end{matrix} \right\rangle \right]^{[\sigma]\theta[\mu]\varphi} . \tag{7-224b}$$

Attaching the Young tableaux $Y^{(\nu')}_{m'}(\omega^0_1)$ and $Y^{(\nu'')}_{m''}(\omega^0_2)$ with $(\omega^0_1) = (1, 2, \ldots, f_1)$ and $(\omega^0_2) = (f_1 + 1, \ldots, f)$ to the two irreducible basis vectors on the right-hand side of (7-224a), it reads:

$$\begin{aligned} \left| \begin{matrix} [\nu] \\ \tau\nu' m' \nu'' m'', \beta\sigma w_1 \mu w_2 \end{matrix} \right\rangle &= \sum_{\substack{\beta'\sigma'\mu'\theta \\ \beta''\sigma''\mu''\varphi}} C^{[\nu]_\tau,\beta[\sigma]\theta[\mu]\varphi}_{\nu'\beta'\sigma'\mu',\nu''\beta''\sigma''\mu''} \\ &\times \left[\left| \begin{matrix} [\nu'] \\ m'\omega^0_1, \beta'\sigma'\mu' \end{matrix} \right\rangle \left| \begin{matrix} [\nu''] \\ m''\omega^0_2, \beta''\sigma''\mu'' \end{matrix} \right\rangle \right]^{[\sigma]_\theta[\mu]_\varphi}_{w_1 w_2} . \end{aligned} \tag{7-227}$$

The left–hand side of (7-227) is still the $SU_{mn} \supset SU_m \times SU_n$ basis. It belongs to the irrep $[\nu]$ of SU_{mn}. According to Theorem 7.1, it must also belong to the irrep $[\nu]$ of the permutation group $S_f(q)$. On the other hand, $[\nu']m'$ and $[\nu'']m''$ on the right–hand side of (7-227) are fixed. Therefore (7-227) is also an $S_f(q) \supset S_{f_1}(q) \otimes S_{f_2}(q)$ basis.

With the help of (7-225), the last factor in (7-227) can be put into the form

$$(I) \equiv \left[\left| \begin{matrix}[\nu'] \\ m'\omega_1^0, \beta'\sigma'\mu'\end{matrix} \right\rangle \left| \begin{matrix}[\nu''] \\ m''\omega_2^0, \beta''\sigma''\mu''\end{matrix} \right\rangle\right]^{[\sigma]_\theta[\mu]_\varphi}_{w_1 w_2}$$

$$= \sum_{w_1' w_2' w_1'' w_2''} C^{[\sigma]\theta, w_1}_{\sigma' w_1', \sigma'' w_1''} C^{[\mu]\varphi, w_2}_{\mu' w_2', \mu'' w_2''} \left| \begin{matrix}[\nu'] \\ m'\omega_1^0, \beta'\sigma' w_1'\mu' w_2'\end{matrix} \right\rangle \left| \begin{matrix}[\nu''] \\ m''\omega_2^0, \beta''\sigma'' w_1''\mu'' w_2''\end{matrix} \right\rangle .$$

Using (7-106a), the $SU_{mn} \supset SU_m \times SU_n$ bases can be further expanded; thus

$$(I) = \sum_{\substack{w_1' w_2' w_1'' w_2'' \\ m_1' m_2' m_1'' m_2''}} C^{[\sigma]\theta, w_1}_{[\sigma']w_1'[\sigma'']w_1''} C^{[\mu]\varphi, w_2}_{[\mu']w_2', [\mu'']w_2''} C^{[\nu']\beta', m'}_{[\sigma']m_1'[\mu']m_2'} C^{[\nu'']\beta'', m''}_{[\sigma'']m_1'', [\mu'']m_2''}$$

$$\times \left| \begin{matrix}[\sigma'] \\ m_1'\omega_1^0, w_1'\end{matrix} \right\rangle \left| \begin{matrix}[\mu'] \\ m_2'\omega_1^0, w_2'\end{matrix} \right\rangle \left| \begin{matrix}[\sigma''] \\ m_1''\omega_2^0, w_1''\end{matrix} \right\rangle \left| \begin{matrix}[\mu''] \\ m_2''\omega_2^0, w_2''\end{matrix} \right\rangle$$

$$= \sum_{m_1' m_2' m_1'' m_2''} C^{[\nu']\beta', m'}_{[\sigma']m_1', [\mu']m_2'} C^{[\nu'']\beta'', m''}_{[\sigma'']m_1'', [\mu'']m_2''} \left| \theta[\sigma']m_1'[\sigma'']m_1'', w_1 \right\rangle \left| \begin{matrix}[\mu] \\ \varphi[\mu']m_2'[\mu'']m_2'', w_2\end{matrix} \right\rangle ,$$

(7-228)

where (7-102b) has been used in the last step. Comparing (4-200) and (4-199) with (7-227) and (7-228), one obtains an important relation,

$$C^{[\nu]\tau, \beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'\sigma'\mu', [\nu'']\beta''\sigma''\mu''} = C^{[\nu]\beta, \tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'', [\mu]\varphi\mu'\mu''} . \qquad (7\text{-}229)$$

$$\mathcal{SU}_{mn} \supset \mathcal{SU}_m \times \mathcal{SU}_n \text{ ISF} \qquad S_{f_1+f_2} \supset S_{f_1} \otimes S_{f_2} \text{ ISF}$$

Expressed in the form of overlap integrals this relation is written as

$$\left\langle \begin{matrix}[\nu] \\ \tau\nu' m'\nu'' m'', \beta\sigma w_1 \mu w_2\end{matrix} \right| \left[\left| \begin{matrix}[\sigma] \\ \theta\sigma'\sigma'', w_1\end{matrix} \right\rangle \left| \begin{matrix}[\mu] \\ \varphi\mu'\mu'', w_2\end{matrix} \right\rangle\right]^{[\nu']_{\beta'}[\nu'']_{\beta''}}_{m'm''} \Bigg\rangle$$

$$= \left\langle \begin{matrix}[\nu] \\ \tau\nu' m'\nu'' m'', \beta\sigma w_1 \mu w_2\end{matrix} \right| \left[\left| \begin{matrix}[\nu'] \\ m', \beta'\sigma'\mu'\end{matrix} \right\rangle \left| \begin{matrix}[\nu''] \\ m'', \beta''\sigma''\mu''\end{matrix} \right\rangle\right]^{[\sigma]_\theta[\mu]_\varphi}_{w_1 w_2} \Bigg\rangle . \qquad (7\text{-}230)$$

Thus we proved that the $SU_{mn} \supset SU_m \times SU_n$ ISF (or the f_2–particle CFP) are just the $S_{f_1+f_2} \supset S_{f_1} \otimes S_{f_2}$ ISF and that the values of the $SU_{mn} \supset SU_m \times SU_n$ ISF do not depend on m and n explicitly, since the values of $S_{f_1+f_2} \supset S_{f_1} \otimes S_{f_2}$ ISF are independent of m and n.

Remark: More precisely, from (7-229) we can only identify the $U_{mn} \supset U_m \times U_n$ CFP with the $S_f \supset S_{f_1} \otimes S_{f_2}$ ISF. However the overall phase convention in Sec. 4.19 ensures that CFP calculated from (7-229) is also the $SU_{mn} \supset SU_m \times SU_n$ CFP (Chen, Gao, Shi 1984).

Setting $[\nu''] = [\sigma''] = [\mu''] = [1]$ in (7-229), ignoring the redundant labels $\tau, \theta, \varphi, \beta'', \sigma''$ and μ'', and using (4-189b), we obtain an expression for the $SU_{mn} \supset SU_m \times SU_n$ one–particle CFP

in terms of the CG coefficients of the permutation groups S_f and S_{f-1},

$$C^{[\nu],\beta\sigma\mu}_{[\nu']\beta'\sigma'\mu',[1]} = C^{[\nu]\beta,[\nu']\beta'}_{[\sigma]\sigma',[\mu]\mu'} = \sum_{m'_1 m'_2} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} C^{[\nu']\beta',m'}_{\sigma' m'_1,\mu' m'_2} \,. \tag{7-231a}$$

When β' is redundant, this reduces to (4-189c), that is,

$$C^{[\nu],\beta\sigma\mu}_{[\nu']\sigma'\mu',[1]} = C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} / C^{[\nu'],m'}_{\sigma' m'_1,\mu' m'_2} \tag{7-231b}$$

The $S_f \supset S_{f-1}$ ISF, or the $SU_{mn} \supset SU_m \times SU_n$ one-body CFP in (7-231b) gives the probability amplitude that the f particles are in the $SU_{mn} \supset SU_m \times SU_n$ state $|[\nu]\beta\sigma\mu\rangle$ after adding the last particle to the state $|[\nu']\beta'\sigma'\mu'\rangle$.

From (7-231a) and (4-196g) we have

$$C^{[1^n][\sigma][\tilde{\sigma}]}_{[1^{n-1}][\sigma'][\tilde{\sigma}'],[1]} = \Lambda^{\sigma}_{\sigma'} \sqrt{h_{\sigma'}/h_{\sigma}} \,. \tag{7-232}$$

7.16.2. The evaluation of the $SU_{mn} \supset SU_m \times SU_n$ many-particle CFP

Making use of (4-168a) and (4-92a), we have

$$\left| \begin{matrix} [\nu]\beta \\ \tau\nu' m' \nu'' m'' \end{matrix} \right\rangle = \sum_{m m_1 m_2}^{\text{fix } m' m''} \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \middle| [\nu], \begin{matrix} \tau\nu'\nu'' \\ m' m'' \end{matrix} \right\rangle C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} \varphi^{\sigma}_{m_1} \psi^{\mu}_{m_2} \,. \tag{7-233}$$

By using the factorization formula (4-189a) of the CG coefficients f_2 times, we get

$$C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} = \sum_{\beta'} I^{\nu m\beta,\nu'\beta'}_{\sigma m_1\sigma',\mu m_2\mu'} C^{[\nu']\beta',m'}_{\sigma' m'_1,\mu' m'_2} \,, \tag{7-234a}$$

where I is a sum of products of the $S_f \supset S_{f-1}$ ISF, $S_{f-1} \supset S_{f-2}$ ISF,... and $S_{f_1+1} \supset S_{f_1}$ ISF,

$$I^{\nu m\beta,\nu'\beta'}_{\sigma m_1\sigma',\mu m_2\mu'} = \sum_{\bar{\beta}\bar{\bar{\beta}}\cdots\widehat{\beta}} C^{\nu\beta,\bar{\nu}\bar{\beta}}_{\sigma\bar{\sigma},\mu\bar{\mu}} C^{\bar{\nu}\bar{\beta},\bar{\bar{\nu}}\bar{\bar{\beta}}}_{\bar{\sigma}\bar{\bar{\sigma}},\bar{\mu}\bar{\bar{\mu}}} \cdots C^{\hat{\nu}\hat{\beta},\nu'\beta'}_{\widehat{\sigma}\sigma',\hat{\mu}\mu'} \,, \tag{7-234b}$$

with $[\sigma]m_1 = [\sigma][\bar{\sigma}][\bar{\bar{\sigma}}]\ldots[\widehat{\sigma}][\sigma']m'_1, [\mu]m_2 = [\mu][\bar{\mu}][\bar{\bar{\mu}}]\ldots[\widehat{\mu}][\mu']m'_2$.

Notice that I depends not only on $\nu, \beta, \nu'\beta', \sigma, \sigma', \mu$ and μ', but also on m_1, m_2 and m, that is, on the positions of the numbers $f, f-1, \ldots, f_1$ in the Young tableaux $Y^{\sigma}_{m_1}, Y^{\mu}_{m_2}$ and Y^{ν}_{m}.

From (7-234a) we have

$$I^{\nu m\beta,\nu'\beta'}_{\sigma m_1\sigma',\mu m_2\mu'} = \sum_{m'_1 m'_2}^{\text{fix } m'} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} C^{[\nu']\beta',m'}_{\sigma' m'_1,\mu' m'_2} \,. \tag{7-234c}$$

Using (4-168b) and (7-234), (7-233) reads

$$\left| \begin{matrix} [\nu]\beta \\ \tau\nu' m' \nu'' m'' \end{matrix} \right\rangle = \sum^{\text{fix } m'_1 m'_2} \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \middle| [\nu], \begin{matrix} \tau\nu'\nu'' \\ m' m'' \end{matrix} \right\rangle \left\langle \begin{matrix} [\sigma] \\ m_1 \end{matrix} \middle| [\sigma], \begin{matrix} \theta\sigma'\sigma'' \\ m'_1 m''_1 \end{matrix} \right\rangle \left\langle \begin{matrix} [\mu] \\ m_2 \end{matrix} \middle| [\mu], \begin{matrix} \varphi\mu'\mu'' \\ m'_2 m''_2 \end{matrix} \right\rangle$$

$$\times I^{\nu m\beta,\nu'\beta'}_{\sigma m_1\sigma',\mu m_2\mu'} \left[\sum_{m'_1 m'_2} C^{[\nu']\beta',m'}_{\sigma' m'_1,\mu' m'_2} \left| \begin{matrix} [\sigma] \\ \theta\sigma' m'_1 \sigma'' m''_1 \end{matrix} \right\rangle \left| \begin{matrix} [\mu] \\ \varphi\mu' m'_2 \mu'' m''_2 \end{matrix} \right\rangle \right] \,, \tag{7-235a}$$

where the first sum runs over $m, m_1, m_2, m''_1, m''_2, \sigma'', \mu'', \beta', \theta$ and φ under fixed m'_1 and m'_2. In deriving (7-235a), we used the independence of the SDC and $I^{\nu m\beta,\nu'\beta'}_{\sigma m_1\sigma',\mu m_2\mu'}$ from m'_1 and m'_2. The square bracket term in (7-235a) can be expressed as

$$\left[\ \right] = \sum_{\nu''\beta''m''} C^{[\nu'']\beta'',m''}_{\sigma'' m''_1,\mu'' m''_2} \left[\left| \begin{matrix} [\sigma] \\ \theta\sigma'\sigma'' \end{matrix} \right\rangle \left| \begin{matrix} [\mu] \\ \varphi\mu'\mu'' \end{matrix} \right\rangle \right]^{[\nu']\beta'[\nu'']\beta''}_{m'm''} \,. \tag{7-235b}$$

Comparing (7-235) with (4-200), and using (7-229) we get

$$C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} = \sum_{m m_1 m_2 m_1'' m_2''}^{\text{fix } m' m'' m_1' m_2''} I^{\nu m\beta,\nu'\beta'}_{\sigma m_1\sigma',\mu m_2\mu'} C^{[\nu'']\beta'',m''}_{\sigma'' m_1'',\mu'' m_2''}$$
$$\times \left\langle \begin{matrix}[\nu]\\ m\end{matrix} \middle| [\nu], \begin{matrix}\tau\nu'\nu''\\ m'm''\end{matrix} \right\rangle \left\langle \begin{matrix}[\sigma]\\ m_1\end{matrix} \middle| [\sigma], \begin{matrix}\theta\sigma'\sigma''\\ m_1'm_1''\end{matrix} \right\rangle \left\langle \begin{matrix}[\mu]\\ m_2\end{matrix} \middle| [\mu] \begin{matrix}\varphi\mu'\mu''\\ m_2'm_2''\end{matrix} \right\rangle . \tag{7-236a}$$

Using (7-234c) this can be rewritten as

$$C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} = \sum_{m m_1 m_2 m_1'' m_2''}^{\text{fix } m' m''} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} C^{[\nu']\beta',m'}_{\sigma' m_1',\mu' m_2'} C^{[\nu'']\beta'',m''}_{\sigma'' m_1'',\mu'' m_2''}$$
$$\times \left\langle \begin{matrix}[\nu]\\ m\end{matrix} \middle| [\nu], \begin{matrix}\tau\nu'\nu''\\ m'm''\end{matrix} \right\rangle \left\langle \begin{matrix}[\sigma]\\ m_1\end{matrix} \middle| [\sigma], \begin{matrix}\theta\sigma'\sigma''\\ m_1'm_1''\end{matrix} \right\rangle \left\langle \begin{matrix}[\mu]\\ m_2\end{matrix} \middle| [\mu] \begin{matrix}\varphi\mu'\mu''\\ m_2'm_2''\end{matrix} \right\rangle . \tag{7-236b}$$

When τ is redundant, (7-236b) can be simplified as,

$$C^{[\nu],\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} = \left\langle \begin{matrix}[\nu]\\ m\end{matrix} \middle| [\nu], \begin{matrix}\nu'\nu''\\ m'm''\end{matrix} \right\rangle^{-1} \sum_{m_1 m_2 m_1'' m_2''}^{\text{fix } m_1' m_2'} I^{\nu m\beta,\nu'\beta'}_{\sigma m_1\sigma',\mu m_2\mu'}$$
$$\times C^{[\nu'']\beta'',m''}_{\sigma'' m_1'',\mu'' m_2''} \left\langle \begin{matrix}[\sigma]\\ m_1\end{matrix} \middle| [\sigma] \begin{matrix}\theta\sigma'\sigma''\\ m_1'm_1''\end{matrix} \right\rangle \left\langle \begin{matrix}[\mu]\\ m_2\end{matrix} \middle| [\mu] \begin{matrix}\varphi\mu'\mu''\\ m_2'm_2''\end{matrix} \right\rangle . \tag{7-237}$$

Equations (7-236a) and (7-237) offer a convenient method for calculating the many–particle CFP from the one–particle CFP and the SDC, while (7-236b) and the following simplified formulas are used to calculate the CFP from the CG coefficients and the SDC of permutation groups.

1. When the multiplicity labels τ and β' are redundant, we have

$$C^{[\nu],\beta[\sigma]\theta[\mu]\varphi}_{\nu'\sigma'\mu',\nu''\beta''\sigma''\mu''} = \left[\left\langle \begin{matrix}[\nu]\\ m\end{matrix} \middle| [\nu], \begin{matrix}\nu'\nu''\\ m'm''\end{matrix} \right\rangle C^{[\nu']m'}_{\sigma' m_1',\mu' m_2'} \right]^{-1}$$
$$\times \sum_{m_1 m_2 m_1'' m_2''}^{\text{fix } m_1' m_2'} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} C^{[\nu'']\beta'',m''}_{\sigma'' m_1'',\mu'' m_2''} \left\langle \begin{matrix}[\sigma]\\ m_1\end{matrix} \middle| [\sigma] \begin{matrix}\theta\sigma'\sigma''\\ m_1'm_1''\end{matrix} \right\rangle \left\langle \begin{matrix}[\mu]\\ m_2\end{matrix} \middle| [\mu] \begin{matrix}\varphi\mu'\mu''\\ m_2'm_2''\end{matrix} \right\rangle . \tag{7-238a}$$

Using the symmetry in (7-242b), the case when φ and β' (or θ and β') are redundant can be converted to the above case.

2. When the multiplicity label β' is redundant, we obtain

$$C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{\nu'\sigma'\mu',\nu''\beta''\sigma''\mu''} = \left(C^{[\nu'],m'}_{\sigma' m_1',\mu' m_2'} \right)^{-1} \sum_{m m_1 m_2}^{\text{fix } m' m'' m_1' m_2'} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} C^{[\nu'']\beta'',m''}_{\sigma'' m_1'',\mu'' m_2''}$$
$$\times \left\langle \begin{matrix}[\nu]\\ m\end{matrix} \middle| [\nu], \begin{matrix}\tau\nu'\nu''\\ m'm''\end{matrix} \right\rangle \left\langle \begin{matrix}[\sigma]\\ m\end{matrix} \middle| [\sigma], \begin{matrix}\theta\sigma'\sigma''\\ m_1'm_1''\end{matrix} \right\rangle \left\langle \begin{matrix}[\mu]\\ m_2\end{matrix} \middle| [\mu], \begin{matrix}\varphi\mu'\mu''\\ m_2'm_2''\end{matrix} \right\rangle . \tag{7-238b}$$

The case when β'' is redundant can be converted to the above case using (7-239a).

For two–particle CFP, (7-236a) and (7-237) reduce to

$$C^{[\nu],\beta\sigma\mu}_{[\nu']\beta'\sigma'\mu',[\nu'']\sigma'\mu''} = \langle [\nu] m | [\nu''] \rangle^{-1} \sum_{m_1 m_2 \overline{\beta}}^{\text{fix } m_1' m_2'} C^{\nu\beta,\overline{\nu}\overline{\beta}}_{\sigma\overline{\sigma},\mu\overline{\mu}} C^{\overline{\nu}\overline{\beta},\nu'\beta'}_{\overline{\sigma}\sigma',\overline{\mu}\mu'} \langle [\sigma] m_1 | [\sigma''] \rangle \langle [\mu] m_2 | [\mu''] \rangle , \tag{7-238c}$$

where $[\nu''] = [\sigma''] \times [\mu'']$, and the simpler notation $\langle [\nu] m | [\nu''] \rangle$ is used for the SDC. Equation (7-238c) is a simplified version of the formula given by Harvey (1981 p. 235) (what he defined as the K coefficients are just the $SU_{mn} \supset SU_m \times SU_n$ ISF).

7.16.3. Symmetries of the $SU_{mn} \supset SU_m \times SU_n$ ISF

From (3-328)–(330a) we obtain the following three symmetries:

1. $$C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} = \varepsilon_1 C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu'']\beta''\sigma''\mu'',[\nu']\beta'\sigma'\mu'} , \tag{7-239a}$$

where ε_1 (or ε_i in the following) is a phase factor, depending on all partitions, $\varepsilon_1 = \pm 1$. For more detailed discussion, see Chen, Wu & Gao (1991).

2. $$C^{[\nu]\tau\beta\sigma\mu}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} = \varepsilon_2 C^{[\overline{\nu}]\tau,\beta\overline{\sigma\mu}}_{[\overline{\nu}']\beta'\overline{\sigma}'\overline{\mu}',[\overline{\nu}'']\beta''\overline{\sigma}''\overline{\mu}''} . \tag{7-239b}$$

3. $$\sqrt{\frac{H_\sigma H_\mu}{H_\nu}} C^{[\nu],\beta\sigma\mu}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} = \varepsilon_3 \sqrt{\frac{H_{\sigma'} H_{\mu'}}{H_{\nu'}}} C^{[\overline{\nu}'],\beta'\overline{\sigma}'\overline{\mu}'}_{[\overline{\nu}]\beta\overline{\sigma\mu},[\nu'']\beta''\sigma''\mu''} , \tag{7-240}$$

where H_σ, H_μ, H_ν are the dimensions of the irreps $[\sigma], [\mu], [\nu]$ of $SU_m, SU_n SU_{mn}$, while $[\overline{\nu}], [\overline{\sigma}]$ and $[\overline{\mu}]$ are the contragredient reps of $[\nu], [\sigma]$ and $[\mu]$, respectively.

4. From (4-121), (4-180a) and (7-236b) we have

$$\begin{aligned} C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} &= \varepsilon_4 C^{[\nu]\tau,\beta[\tilde{\sigma}]\theta[\tilde{\mu}]\varphi}_{[\nu']\beta'\tilde{\sigma}'\tilde{\mu}',[\nu'']\beta''\tilde{\sigma}''\tilde{\mu}''} = \varepsilon_5 C^{[\tilde{\nu}]\tau,\beta[\tilde{\sigma}]\theta[\mu]\varphi}_{[\tilde{\nu}']\beta'\tilde{\sigma}'\mu',[\tilde{\nu}'']\beta''\tilde{\sigma}''\mu''} \\ &= \varepsilon_6 C^{[\tilde{\nu}]\tau,\beta[\sigma]\theta[\tilde{\mu}]\varphi}_{[\tilde{\nu}']\beta'\sigma'\tilde{\mu}',[\tilde{\nu}'']\beta''\sigma''\tilde{\mu}''} . \end{aligned} \tag{7-241}$$

where, for example, $[\tilde{\sigma}]$ is the conjugate of the Young diagram $[\sigma]$.

5. We first rewrite (7-236b) in the following form,

$$\begin{aligned} C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} = \frac{1}{h_{\nu'} h_{\nu''}} \sum_{m'm''} \sum_{mm_1m_2m_1''m_2''} & C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} C^{[\nu']\beta',m'}_{\sigma' m_1',\mu m_2'} C^{[\nu'']\beta'',m''}_{\sigma'' m_1'',\mu'' m_2''} \\ \times \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \middle| [\nu], \begin{matrix} \tau\nu'\nu'' \\ m'm'' \end{matrix} \right\rangle & \left\langle \begin{matrix} [\sigma] \\ m_1 \end{matrix} \middle| [\sigma] \begin{matrix} \theta\sigma'\sigma'' \\ m_1'm_1'' \end{matrix} \right\rangle \left\langle \begin{matrix} [\mu] \\ m_2 \end{matrix} \middle| [\mu] \begin{matrix} \varphi\mu'\mu'' \\ m_2'm_2'' \end{matrix} \right\rangle . \end{aligned} \tag{7-242a}$$

From (4-177) and (7-242a) it can be shown that

$$\begin{aligned} \sqrt{\frac{h_{\nu'} h_{\nu''}}{h_\nu}} C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} &= \varepsilon_7 \sqrt{\frac{h_{\sigma'} h_{\sigma''}}{h_\sigma}} C^{[\sigma]\theta,\beta[\nu]\tau[\mu]\varphi}_{[\sigma']\beta'\nu'\mu',[\sigma'']\beta''\nu''\mu''} \\ &= \varepsilon_8 \sqrt{\frac{h_{\mu'} h_{\mu''}}{h_\mu}} C^{[\mu]\varphi,\beta[\sigma]\theta[\nu]\tau}_{[\mu']\beta'\sigma'\nu',[\mu'']\beta''\sigma''\nu''} , \end{aligned} \tag{7-242b}$$

where, for example, h_ν is the dimension of the irrep $[\nu]$ of S_f.

6. $$C^{[\nu]\beta,[\sigma][\mu]}_{[\nu']\beta'[\sigma'][\mu'],[0][0][0]} = \delta_{\nu\nu'}\delta_{\beta\beta'}\delta_{\sigma\sigma'}\delta_{\mu\mu'} . \tag{7-243a}$$

$$C^{[0],[0][0]}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} = \sqrt{\frac{H_{\sigma'} H_{\mu'}}{H_{\nu'}}} \delta_{\nu'\overline{\nu}''}\delta_{\beta'\beta''}\delta_{\sigma'\overline{\sigma}''}\delta_{\mu'\overline{\mu}''} . \tag{7-243b}$$

7. From (4-203) and (4-204) we have

$$C^{[\nu]\tau,[f][\mu]\varphi}_{[\nu'][f_1][\mu'],[\nu''][f_2][\mu'']} = \delta_{\nu\mu}\delta_{\nu'\mu'}\delta_{\nu''\mu''}\delta_{\tau\varphi} . \tag{7-243c}$$

$$C^{[\nu]\tau,[1^f][\mu]\varphi}_{[\nu'][1^{f_1}][\mu'],[\nu''][1^{f_2}][\mu'']} = \delta_{\nu\tilde{\mu}}\delta_{\nu'\tilde{\mu}'}\delta_{\nu''\tilde{\mu}''}\delta_{\tau\varphi} . \tag{7-243d}$$

8. From (7-236b), (4-180a), (4-171b) and (4-124), we obtain

$$C^{[f],[\sigma]\theta[\mu]\varphi}_{[f_1]\sigma'\mu',[f_2]\sigma''\mu''} = \sqrt{\frac{h_{\sigma'}h_{\sigma''}}{h_\sigma}}\delta_{\sigma\mu}\delta_{\sigma'\mu'}\delta_{\sigma''\mu''}\delta_{\theta\varphi} \ . \tag{7-244a}$$

$$C^{[1^f],[\sigma]\theta[\mu]\varphi}_{[1^{f_1}]\sigma'\mu',[1^{f_2}]\sigma''\mu''} = \varepsilon_3(\sigma'\sigma''\sigma_\theta)\sqrt{\frac{h_{\sigma'}h_{\sigma''}}{h_\sigma}}\delta_{\sigma\tilde{\mu}}\delta_{\sigma'\tilde{\mu}'}\delta_{\sigma''\tilde{\mu}''}\delta_{\theta\varphi} \ . \tag{7-244b}$$

The symmetries (7-239), (7-240) and (7-243a, b) come from the unitary group, while the symmetries (7-241), (7-242), (7-243c,d) and (7-244) come from the permutation group. It is seen that the interplay of these two groups greatly deepens our understanding of the symmetries of the ISF of the two groups. For example, for the $SU_4 \supset SU_2 \times SU_2$ ISF, we obtain from (7-239b) and (7-240)

$$\begin{aligned} C^{[221][41][32]}_{[21][3][21],[2][2][2]} &= \varepsilon_2 C^{[4322][74][65]}_{[221][41][32],[222][42][42]} \\ &= \varepsilon_3' \left(\sqrt{\frac{3\times 3}{H_{[222]}(SU_4)}} \Big/ \sqrt{\frac{4\times 2}{H_{[221]}(SU_4)}} \right) C^{[222][42][42]}_{[21][3][21],[21][3][21]} \ . \end{aligned}$$

Here the equivalence (7-71) has been used. It is seen that the two–particle CFP for a five–particle system, and the six–particle CFP for an eleven–particle system, and the three–particle CFP for a six–particle system are related to one another. This cannot be understood from the point of view of the permutation group. $C^{[221][41][32]}_{[21][3][21],[2][2][2]}$ is also the $SU_6 \supset SU_3 \times SU_2$ ISF, therefore it also has the following symmetries:

$$\begin{aligned} C^{[221][41][32]}_{[21][3][21],[2][2][2]} &= \varepsilon_4 C^{[4^3 3 2^2][874][10,9]}_{[2^4 1][4^2 1][54],[2^5][4^2 2][64]} \\ &= \varepsilon_3 \left(\sqrt{\frac{2H_{[33]}(SU_3)}{H_{[2^4 1]}(SU_6)}} \Big/ \sqrt{\frac{2H_{[41]}(SU_3)}{H_{[221]}(SU_6)}} \right) C^{[2^4 1][4^2 1][54]}_{[2^3 1][43][43],[2][2][2]} \ . \end{aligned}$$

Example 1: The application of (7-244b). The $SU_{12} \supset SU_4 \times SU_3$ ISF, evaluated with much labor by Matveev (1978), can be easily found from (7-244b) (under the convention $\varepsilon_3 = 1$):

$$\begin{aligned} C^{[1^6][33][\widetilde{33}]}_{[1^3][3][\tilde{3}],[1^3][3][\tilde{3}]} &= \sqrt{h_{[3]}h_{[3]}/h_{[33]}} = \sqrt{1/5} \ , \\ C^{[1^6][33][\widetilde{33}]}_{[1^3][21][21],[1^3][21][21]} &= \sqrt{h_{[21]}h_{[21]}/h_{[33]}} = \sqrt{4/5} \ . \end{aligned}$$

7.16.4. More examples

We use the following examples to check the validity of the conclusion that the $SU_{mn} \supset SU_m \times SU_n$ ISF do not depend on m and n explicitly.

Example 2: Single–particle CFP. The $SU_{mn} \supset SU_m \times SU_n$ single–particle CFP are listed in Table 4.19 for particle number $f \leq 5$, and in Chen, Gao, Shi (1984) for $f \leq 6$.

Table 4.19-13d is reproduced in Table 7.16, supplemented with the headings for the $SU_4 \supset SU_2 \times SU_2$ and $SU_6 \supset SU_3 \times SU_2$ CFP. It is seen that except for the phase, the $SU_{mn} \supset SU_m \times SU_n$ CFP listed in Table 7.16 are identical not only with the $SU_4 \supset SU_2 \times SU_2$ CFP (Jahn 1951) but also with the $SU_6 \supset SU_3 \times SU_2$ CFP (So 1979). The phase in Jahn's $SU_4 \supset SU_2 \times SU_2$ CFP has not been systematically determined. In Sec. 4.19 we gave a systematic way to determine the phase of the $SU_{mn} \supset SU_m \times SU_n$ ISF.

Example 3: Two–particle CFP. We can use (7-238c) to find a particular two–particle CFP, $C^{[221],[41][32]}_{[21][3][21],[2][2][2]}$. The value m in (7-238c) can be chosen arbitrarily. We take $m = 1$, that is

Table 7.16. $SU_4 \supset SU_2 \times SU_2$ ISF $C^{[\nu],ST}_{[\nu'],S'T',[1]}$
$SU_6 \supset SU_3 \times SU_2$ ISF $C^{[\nu],(\lambda\mu)S}_{[\nu'],(\lambda'\mu')S',[1]}$
$SU_{mn} \supset SU_m \times SU_n$ ISF $C^{[\nu],\sigma\mu}_{[\nu']\sigma'\mu',[1]}$

$SU_4 \supset SU_2 \times SU_2$	$SU_6 \supset SU_3 \times SU_2$	$SU_{mn} \supset SU_m \times SU_n$	$[\nu'] = [211]$
${}^{2S+1,2T+1}\Gamma$	$(\lambda\mu)S$	$[\sigma]$ $[\mu]$	$[\nu]$
${}^{22}\Gamma$	(12)1/2	[32] [32]	[311] [221] [211]
${}^{2S'+1,2T'+1}\Gamma$	$(\lambda'\mu')S'$	$[\sigma']$ $[\mu']$	
${}^{23}\Gamma$	(21)1	[31] [31]	$\sqrt{2/5}$ 0 $\sqrt{3/5}$
${}^{31}\Gamma$	(21)0	[31] [22]	$\sqrt{3/10}$ $\sqrt{1/2}$ $-\sqrt{1/5}$
${}^{13}\Gamma$	(02)1	[22] [31]	$-\sqrt{3/10}$ $\sqrt{12}$ $\sqrt{15}$

$[221]m = \begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\hline 5\\\cline{1-1}\end{array}$. Therefore

$$C^{[221],[41][32]}_{[21][3][21],[2][2][2]} = \left\langle \begin{matrix}1\,2\\3\,4\\5\end{matrix} \middle| [2] \right\rangle^{-1}$$
$$\times \left\{ \left\langle \begin{matrix}1\,2\,3\,4\\5\end{matrix} \middle| [2] \right\rangle \left\langle \begin{matrix}1\,2\,4\\3\,5\end{matrix} \middle| [2] \right\rangle C^{[221][22]}_{[41][4],[32][31]} C^{[22][21]}_{[4][3],[31][21]} \right.$$
$$+ \left\langle \begin{matrix}1\,2\,3\,5\\4\end{matrix} \middle| [2] \right\rangle \left\langle \begin{matrix}1\,2\,4\\3\,5\end{matrix} \middle| [2] \right\rangle C^{[221][22]}_{[41][31],[32][31]} C^{[22][21]}_{[31][3],[31][21]}$$
$$+ \left\langle \begin{matrix}1\,2\,3\,4\\5\end{matrix} \middle| [2] \right\rangle \left\langle \begin{matrix}1\,2\,5\\3\,4\end{matrix} \middle| [2] \right\rangle C^{[221][22]}_{[41][4],[32][22]} C^{[22],[21]}_{[4][3],[22][21]}$$
$$\left. + \left\langle \begin{matrix}1\,2\,3\,5\\4\end{matrix} \middle| [2] \right\rangle \left\langle \begin{matrix}1\,2\,5\\3\,4\end{matrix} \middle| [21] \right\rangle C^{[221][22]}_{[41][31],[32][22]} C^{[22][21]}_{[31][3],[22][21]} \right\} .$$

Using the formula (4-184) and one-body ISF Table 4.19, we obtain

$$C^{[221][41][32]}_{[21][3][21],[2][2][2]} = 2\left\{0 + \sqrt{\tfrac{5}{8}}\sqrt{\tfrac{1}{4}}\left(-\sqrt{\tfrac{3}{8}}\right)\sqrt{\tfrac{1}{3}} + \sqrt{\tfrac{3}{8}}\sqrt{\tfrac{3}{4}}\sqrt{\tfrac{5}{8}}(1) + 0\right\} = \sqrt{\tfrac{5}{16}}\,.$$

This is seen to be identical, to within a phase factor, to the $SU_4 \supset SU_2 \times SU_2$ CFP tabulated by Elliott (1953),

$$C^{[221],[41][32]}_{[21][3][21],[2][2][2]} = C^{[\widetilde{32}]^{42}\Gamma}_{[21]^{42}\Gamma,[2]^{33}\Gamma} = \sqrt{\tfrac{5}{16}}\,.$$

In summary, the values of the $SU_{mn} \supset SU_m \times SU_n$ CFP depend only on the partitions rather than on m and n. The reason we failed to recognize this is because we usually use specific quantum numbers for a given m and n instead of partitions to label the irreps of SU_m and SU_n. Now we know that each $SU_{mn} \supset SU_m \times SU_n$ CFP with a particular m and n gives an infinite number of $SU_{m'n'} \supset SU_{m'} \times SU_{n'}$ CFP with $m' = m, m+1, \ldots$ and $n' = n, n+1, \ldots$. However, not every $SU_{mn} \supset SU_m \times SU_n$ CFP can be deduced from the $SU_{(m-1)n} \supset SU_{m-1} \times SU_n$ CFP or $SU_{m(n-1)} \supset SU_m \times SU_{n-1}$ CFP. This is because the groups SU_m and SU_n have more possible partitions than the groups SU_{m-1} and SU_{n-1}. The partitions of SU_m can have at most m rows, while those of SU_{m-1}, only $m-1$ rows. Therefore the $SU_{mn} \supset SU_m \times SU_n$ CFP with $[\sigma'], [\sigma'']$ of $[\sigma]$ of m rows cannot be deduced from the $SU_{(m-1)n} \supset SU_{m-1} \times SU_n$ CFP.

At long last we give an example to illustrate the use of (7-238a).

Example 4: Find the three-particle CFP $A = C^{[21^4][222][41]}_{[1^3][21][21],[1^3][21][21]}$. In applying (7-238a), the indices m_1, m_2, m', m'' and m can be chosen arbitrarily. A suitable choice will reduce the

labor involved in the calculation. We take $m_1' = 1, m_2' = 2$ and $m = 5$. From (7-238a) we have

$$A = \left(\left\langle \begin{matrix} [21^4] \\ 5 \end{matrix} \middle| [1^3][1^3] \right\rangle \sqrt{1/2} \right)^{-1} \sum_{m_1 m_2 m_1'' m_2''} C^{[21^4]5}_{[222]m_1,[42]m_2} \times \left\langle \begin{matrix} [222] \\ m_1 \end{matrix} \middle| \begin{matrix} [21] & [21] \\ 1 & m_1'' \end{matrix} \right\rangle \left\langle \begin{matrix} [42] \\ m_2 \end{matrix} \middle| \begin{matrix} [21] & [21] \\ 2 & m_2'' \end{matrix} \right\rangle C^{[1^3]}_{[21]m_1'',[21]m_2''} .$$

Using the symmetries (4-122) and (4-180a), as well as the CG coefficients of S_3, we get

$$A = \left\langle \begin{matrix} [51] \\ 1 \end{matrix} \middle| [3][3] \right\rangle^{-1} \sum_{m_1 m_2 m_2''} C^{[51]1}_{[33]m_1,[42]m_2} \left\langle \begin{matrix} [33] \\ m_1 \end{matrix} \middle| \begin{matrix} [21] & [21] \\ 2 & m_2'' \end{matrix} \right\rangle \left\langle \begin{matrix} [42] \\ m_2 \end{matrix} \middle| \begin{matrix} [21] & [21] \\ 2 & m_2'' \end{matrix} \right\rangle .$$

From Table 4.18 we know the ranges of m_1 and m_2; $m_1 = 3, 5, m_2 = 4, 7, 9$. From the table of CG coefficients (Chen & Gao 1981), $C^{[51]1}_{[33]3,[42]7} = C^{[51]1}_{[33]5,[42]9} = \sqrt{1/5}$. we finally obtain

$$C^{[\widetilde{51}],[222][41]}_{[1^3][21][21],[1^3][21][21]} = \frac{2}{3} .$$

All the $SU_{mn} \supset SU_m \times SU_n$ CFP have been tabulated in Chen, Wu & Gao (1991) for systems with up to 6 particles.

7.16.5. $SU_{4(2l+1)} \supset (SU_{2l+1} \supset SO_3) \times (SU_4 \supset SU_2 \times SU_2)$ ISF and total CFP

Equation (7-185) already gives an expression between the total CFP and the ISF. Now let us further consider the problem of constructing wave functions for a system of f particles with a definite symmetry $[\nu]$ under the $SU_{4(2l+1)}$ transformations, out of the totally anti-symmetric wave functions of the subsystems with f_1 and f_2 particles. To simplify notations, we ignore the additional labels α and β (or equivalently, we absorb α and β into the labels L and ST, respectively). Suppose

$$\left| \begin{matrix} [\nu] \\ \varepsilon[\sigma]L[\mu]ST \end{matrix} \right\rangle \quad \text{belong to} \quad \begin{matrix} SU_{4(2l+1)} \supset (SU_{2l+1} \supset SO_3) \times (SU_4 \supset SU_2 \times SU_2) \\ [\nu] \qquad\quad [\sigma] \qquad L \qquad [\mu] \qquad S \qquad T \end{matrix} , \tag{7-245}$$

where $\varepsilon = 1, 2, \ldots, (\sigma\mu\nu)$. By means of the ISF, the basis in (7-245) can be expressed in terms of the totally anti-symmetric states of the f_1 and f_2 particles

$$\left| \begin{matrix} [\nu]_\tau \\ \varepsilon[\sigma]L,[\mu]ST \end{matrix} \right\rangle = \sum_{\substack{\sigma' L' S' T' \\ \sigma'' L'' S'' T''}} C^{[\nu]\tau,\varepsilon[\sigma]L[\mu]ST}_{[1^{f_1}]\sigma' L\tilde{\sigma}' S' T',[1^{f_2}]\sigma'' L'' \tilde{\sigma}'' S'' T''} \times \left[\left| \begin{matrix} [1^{f_1}] \\ [\sigma']L'[\tilde{\sigma}']S'T' \end{matrix} \right\rangle \left| \begin{matrix} [1^{f_2}] \\ [\sigma'']L''[\tilde{\sigma}'']S''T'' \end{matrix} \right\rangle \right]^{LST} , \tag{7-246a}$$

where the index τ is redundant, since from the outer-product reduction rule $\{[1^{f_1}][1^{f_2}][\nu]\} \leq 1$. The coefficients in (7-246a) are the $SU_{4(2l+1)} \supset (SU_{2l+1} \supset SO_3) \times (SU_4 \supset SU_2 \times SU_2)$ ISF and they can be factorized as

$$C^{[\nu],\varepsilon[\sigma]L,[\mu]ST}_{[1^{f_1}]\sigma' L'\tilde{\sigma}' S' T',[1^{f_2}]\sigma'' L'' \tilde{\sigma}'' S'' T''} = \sum_{\theta\varphi} C^{[\nu],\varepsilon[\sigma]_\theta[\mu]_\varphi}_{[1^{f_1}]\sigma'\tilde{\sigma}',[1^{f_2}]\sigma''\tilde{\sigma}''} C^{[\sigma]_\theta,L}_{[\sigma']L',[\sigma'']L''} C^{[\mu]_\varphi,ST}_{[\tilde{\sigma}']S'T',[\tilde{\sigma}'']S''T''} . \tag{7-247}$$

The first factor on the right-hand side is the $SU_{4(2l+1)} \supset SU_{2l+1} \times SU_4$ ISF.

Setting $\Lambda \to \mathrm{LST}$ and $\beta \to \varepsilon\sigma\mu$ in (3-307), we obtain the inverse of (7-246a),

$$\left[\left|\begin{matrix}[1^{f_1}]\\ [\sigma']L',[\tilde{\sigma}']S'T'\end{matrix}\right\rangle\left|\begin{matrix}[1^{f_2}]\\ [\sigma'']L'',[\tilde{\sigma}'']S''T''\end{matrix}\right\rangle\right]^{LST}$$

$$= \sum_{\nu\varepsilon\sigma\mu} C^{[\nu],\varepsilon[\sigma]L[\mu]ST}_{[1^{f_1}]\sigma'L'\tilde{\sigma}'S'T',[1^{f_2}]\sigma''L''\tilde{\sigma}''S''T''} \left|\begin{matrix}[\nu]\\ \varepsilon[\sigma]L,[\mu]ST\end{matrix}\right\rangle , \tag{7-246b}$$

where the product of the totally anti-symmetric states of f_1 and f_2 particles is expressed in terms of the states of the f_1+f_2 particles. Notice that the sum in (7-246b) runs over all possible $[\nu]$, instead of only the anti-symmetric term $[1^f]$. One generally uses

$$(l^{f_1}[\sigma']L'S'T', l^{f_2}[\sigma'']L''S''T''|\}l^f[\sigma]LST)$$

to designate the total CFP, with the symbol $(|\})$ stressing the non-unitarity of the total CFP. It is now seen that the total CFP is a special case of the ISF of (7-247) with $[\nu] = [1^f]$ and $[\mu] = [\tilde{\sigma}]$,

$$(l^{f_1}[\sigma']L'S'T', l^{f_2}[\sigma'']L''S''T''|\}l^f[\sigma]LST) = C^{[1^f],[\sigma]L[\tilde{\sigma}]ST}_{[1^{f_1}]\sigma'L'\tilde{\sigma}'S'T';[1^{f_2}]\sigma''L''\tilde{\sigma}''S''T''}, \tag{7-248}$$

while the $SU_{4(2l+1)} \supset (SU_{2l+1} \supset SO_3) \times (SU_4 \supset SU_2 \times SU_2)$ ISF of (7-247) satisfy unitarity.

7.17 The $\mathbf{SU}_{m+n} \supset \mathbf{SU}_m \otimes \mathbf{SU}_n$ CFP*

The remark in the beginning of Sec. 7.16 also applies to the $SU_{m+n} \supset SU_m \otimes SU_n$ CFP. We can now prove that: (a) the $S_{f_1+f_2} \supset S_{f_1} \otimes S_{f_2}$ outer-product ISF are the $SU_{m+n} \supset SU_m \otimes SU_n$ CFP for separating f_2 particles; (b) the values of the $SU_{m+n} \supset SU_m \otimes SU_n$ CFP are thus independent of m and n; (c) the $SU_{m+n} \supset SU_m \otimes SU_n$ CFP can be expressed in terms of the IDC and SDC of the permutation group.

7.17.1 The $S_f \supset S_{f-1}$ outer-product ISF (The $SU_f \supset SU_{f-1} \otimes U_1$ ISF)

In parallel to subsection 4.19.1, the question we are facing now is how to calculate the IDC of S_f if those of S_{f-1} are known. In analogy with Table 4.19-1, we introduce the following notations to designate the irreducible bases of the unitary groups and permutation groups.

Table 7.17-1. Notation for the irreducible bases of S_f and SU_f.

SU_f $S_{f_1}(\omega_1)$ $(\omega_1) = (\omega_1' f)$	SU_{f-1} $S_{f_1-1}(\omega_1')$	SU_f $S_{f_2}(\omega_2)$ $(\omega_2) = (\omega_2' f)$	SU_{f-1} $S_{f_2-1}(\omega_2')$	SU_f S_f	SU_{f-1} S_{f-1}
$\left\|\begin{matrix}[\sigma]\\ m_1\omega_1\end{matrix}\right\rangle = \left\|\begin{matrix}[\sigma]\\ [\sigma']m_1'\omega_1'\end{matrix}\right\rangle$	$\left\|\begin{matrix}[\sigma']\\ m_1'\omega_1'\end{matrix}\right\rangle$	$\left\|\begin{matrix}[\mu]\\ m_2\omega_2\end{matrix}\right\rangle = \left\|\begin{matrix}[\mu]\\ [\mu']m_2'\omega_2'\end{matrix}\right\rangle$	$\left\|\begin{matrix}[\mu']\\ m_2'\omega_2'\end{matrix}\right\rangle$	$\left\|\begin{matrix}[\nu]\\ m\end{matrix}\right\rangle = \left\|\begin{matrix}[\nu]\\ [\nu']m'\end{matrix}\right\rangle$	$\left\|\begin{matrix}[\mu']\\ m'\end{matrix}\right\rangle$

As with (4-186) we have

$$[\sigma]m_1\omega_1 = [\sigma][\sigma']m_1'\omega_1' , \quad [\mu]m_2\omega_2 = [\mu][\mu']m_2'\omega_2' , \quad [\nu]m = [\nu][\nu']m' . \tag{7-249}$$

However, we now have to distinguish between two cases: since the particle index f is either in (ω_1), or in (ω_2). Suppose that f is in (ω_1), then after deleting the box f, the generalized Young tableau $\left|\begin{matrix}\sigma\\ m_1\omega_1\end{matrix}\right\rangle$ goes over to $\left|\begin{matrix}\sigma'\\ m_1'\omega_1'\end{matrix}\right\rangle$, otherwise, it remains $\left|\begin{matrix}\sigma\\ m_1\omega_1\end{matrix}\right\rangle$. For example

$$\left|\begin{matrix}[\sigma]\\ m_1\omega_1\end{matrix}\right\rangle = \left|\begin{matrix}[21]\\ m_1=1,\omega=(135)\end{matrix}\right\rangle = \left|\begin{matrix}\boxed{1}\boxed{3}\\ \boxed{5}\end{matrix}\right\rangle \xrightarrow{\text{delete } 6} \left|\begin{matrix}[\sigma']\\ m_1'\omega_1'\end{matrix}\right\rangle = \left|\begin{matrix}[\sigma]\\ m_1\omega_1\end{matrix}\right\rangle \tag{7-250a}$$

$$\left|\begin{matrix}[\sigma]\\ m_1\omega_1\end{matrix}\right\rangle = \left|\begin{matrix}[21]\\ m_1=2,\ (\omega)=(256)\end{matrix}\right\rangle = \left|\begin{array}{|c|c|}\hline 2&6\\\hline 5\\\cline{1-1}\end{array}\right\rangle \xrightarrow{\text{delete } 6} \left|\begin{array}{|c|}\hline 2\\\hline 5\\\cline{1-1}\end{array}\right\rangle$$

$$= \left|\begin{matrix}[\sigma']\\ m_1'\omega_1'\end{matrix}\right\rangle = \left|\begin{matrix}[11]\\ m_1'=1,\ \omega_1'=(25)\end{matrix}\right\rangle . \tag{7-250b}$$

We first use the IDC of S_{f-1} (the CG coefficients of SU_{f-1}), $C^{[\nu']\beta',m'}_{\sigma' m_1'\omega_1',\mu' m_2'\omega_2'}$, to combine the irreducible bases of $S_{f_1}(\omega_1)$ and $S_{f_2}(\omega_2)$ (the SU_f Gel'fand bases) into the standard basis $[\nu']m'$ of S_{f-1} (the SU_{f-1} Gel'fand basis),

$$|(\sigma'\mu')\beta'\rangle \equiv \left[\left|\begin{matrix}[\sigma]\\ [\sigma']\end{matrix}\right\rangle \left|\begin{matrix}[\mu]\\ [\mu']\end{matrix}\right\rangle\right]^{[\nu']\beta}_{m'} = \sum_{m_1'\omega_1' m_2'\omega_2'} C^{[\nu']\beta',m'}_{\sigma' m_1'\omega_1',\mu' m_2'\omega_2'} \left|\begin{matrix}[\sigma]\\ [\sigma']m_1'\omega_1'\end{matrix}\right\rangle \left|\begin{matrix}[\mu]\\ [\mu']m_2'\omega_2'\end{matrix}\right\rangle . \tag{7-251}$$

We then use the $S_f \supset S_{f-1}$ *outer-product ISF* $C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'}$ to combine (7-251) linearly into the irreducible basis of S_f (the special Gel'fand basis of SU_f),

$$\left|\begin{matrix}[\nu]\beta\\ m\end{matrix}\right\rangle = \left|\begin{matrix}[\nu]\beta\\ [\nu']m'\end{matrix}\right\rangle = \sum_{\sigma'\mu'\beta'} C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'} \left[\left|\begin{matrix}[\sigma]\\ [\sigma']\end{matrix}\right\rangle \left|\begin{matrix}[\mu]\\ [\mu']\end{matrix}\right\rangle\right]^{[\nu']\beta}_{m'} . \tag{7-252}$$

Equation (7-252) has the same form as (4-188), and its inverse expansion is identical to (4-190). Comparing (7-251) and (7-252) with (4-141), and noting that the sum over $\sigma' m_1'\omega_1'$ and $\mu' m_2'\omega_2'$ are equivalent to the sum over $m_1\omega_1$ and $m_2\omega_2$, respectively, we get the factorization formula for the IDC of S_f

$$C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2,\omega} = \sum_{\beta'} C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'} C^{[\nu']\beta' m'}_{\sigma' m_1',\mu' m_2',\omega'} , \tag{7-253}$$

where $(\omega) = (\omega_1, \omega_2)$ and $(\omega') = (\omega_1', \omega_2')$, and the quantum numbers have to satisfy (7-249).

Since the left-hand side contains the SU_f CG coefficients, and the last factor in (7-253) is the SU_{f-1} CG coefficient, the $S_f \supset S_{f-1}$ outer-product ISF are just the $SU_f \supset SU_{f-1}$ ISF. From (7-253) we obtain

$$C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'} = \sum_{m_1' m_2'\omega'} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2,\omega} C^{[\nu']\beta',m'}_{\sigma' m_1',\mu' m_2',\omega'} . \tag{7-254a}$$

When the multiplicity label β' is redundant, from (7-253) we get

$$C^{[\nu]\beta,[\nu']}_{\sigma\sigma',\mu\mu'} = C^{[\nu]\beta.m}_{\sigma m_1,\mu m_2,\omega} / C^{[\nu'],m'}_{\sigma' m_1',\mu' m_2',\omega'} . \tag{7-254b}$$

For example from (7-254b) and Table 4.17-5d and Table 8f(1) of IDC (Chen & Gao 1981) we have

$$C^{[321]\alpha,[311]}_{[21][2],[21][21]} = \left\langle (\alpha)\ \begin{array}{|c|c|c|}\hline 1&3&5\\\hline 2&6\\\cline{1-2} 4\\\cline{1-1}\end{array}\ \middle|\ \begin{array}{|c|c|}\hline 1&3\\\hline 6\\\cline{1-1}\end{array}, \begin{array}{|c|c|}\hline 2&4\\\hline 5\\\cline{1-1}\end{array}\right\rangle \Bigg/ \left\langle \begin{array}{|c|c|c|}\hline 1&3&5\\\hline 2\\\cline{1-1} 4\\\cline{1-1}\end{array}\ \middle|\ \begin{array}{|c|c|}\hline 1&3\\\hline\end{array}, \begin{array}{|c|c|}\hline 2&4\\\hline 5\\\cline{1-1}\end{array}\right\rangle$$

$$= \sqrt{\frac{48}{3480}} \Bigg/ \sqrt{\frac{48}{320}} = \sqrt{\frac{1}{12}} .$$

$$C^{[321]\beta,[32]}_{[21][21],[21][2]} = \left\langle (\beta)\ \begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3&5\\\cline{1-2} 6\\\cline{1-1}\end{array}\ \middle|\ \begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}, \begin{array}{|c|c|}\hline 4&5\\\hline 6\\\cline{1-1}\end{array}\right\rangle \Bigg/ \left\langle \begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3&5\\\cline{1-2}\end{array}\ \middle|\ \begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}, \begin{array}{|c|c|}\hline 4&5\\\hline\end{array}\right\rangle$$

$$= -\sqrt{\frac{48}{768}} \Bigg/ \sqrt{\frac{48}{320}} = -\sqrt{\frac{5}{12}} .$$

Using (4-163b) and (7-254b) we can derive expressions of the $S_{m+n} \supset S_{m+n-1}$ outer-product ISF for the totally antisymmetric case. Let $N = m + n$, and

$$\begin{aligned} \omega_0 &= (1, 2, \cdots, m; m+1, \cdots, N) \\ \omega &= (1, 2, \cdots, m-1, N; m, m+1, \cdots, N-1). \end{aligned} \tag{7-255a}$$

To bring the index N in ω_0 to be behind $m-1$ we need to move the index N across the n indices, $N-1, N-2, \cdots, m$. Therefore $\delta_\omega = (-1)^n$. From (4-163b) we have

$$C^{[1^N]}_{[1^m](1,2,\cdots,m-1,N),[1^n](m,m+1,\cdots,N-1)} \equiv A = (-1)^n \binom{m+n}{m}^{-1/2} \tag{7-255b}$$

From (4-163b) we have the IDC of S_{N-1}

$$C^{[1^{N-1}]}_{[1^{m-1}](1,2,\cdots,m-1),[1^n](m,m+1,\cdots,N-1)} \equiv B = \binom{m+n-1}{m-1}^{-1/2}. \tag{7-255c}$$

Using (7-254b) and (7-255b,c) we get the $S_{m+n} \supset S_{m+n-1}$ outer-product ISF,

$$C^{[1^N],[1^{N-1}]}_{[1^m][1^{m-1}],[1^n][1^n]} = \frac{A}{B} = (-1)^n \sqrt{\frac{m}{m+n}}. \tag{7-255d}$$

Similarly we have

$$C^{[1^N],[1^{N-1}]}_{[1^m][1^m],[1^n][1^{n-1}]} = \sqrt{\frac{n}{m+n}}. \tag{7-255e}$$

The $S_f \supset S_{f-1}$ outer-product ISF still satisfies (4-196a) and the eigenequation (4-192). Equations (4-193) and (4-195) remain true under the following replacements: $n \to f$ and

$$\begin{aligned} &\langle (\overline{\sigma}'\overline{\mu}')\overline{\beta}' | (f-1, f) | (\sigma'\mu')\beta' \rangle \\ &= \sum_{\overline{m}'_1 \overline{m}'_2 \overline{\omega}' m'_1 m'_2 \omega'} C^{[\nu']\beta',m'}_{\overline{\sigma}'\overline{m}'_1,\overline{\mu}'\overline{m}'_2,\overline{\omega}'} C^{[\nu']\beta',m'}_{\sigma' m'_1,\mu' m'_2,\omega'} \langle \overline{m}_1 \overline{m}_2 \overline{\omega} | (f-1, f) | m_1 m_2 \omega \rangle , \end{aligned} \tag{7-256a}$$

where

$$\langle \overline{m}_1 \overline{m}_2 \overline{\omega} | (f-1, f) | m_1 m_2 \omega \rangle = \langle \psi^{[\sigma]}_{\overline{m}_1}(\overline{\omega}_1) \psi^{[\mu]}_{\overline{m}_2}(\overline{\omega}_2) | (f-1, f) | \psi^{[\sigma]}_{m_1}(\omega_1) \psi^{[\mu]}_{m_2}(\omega_2) \rangle , \tag{7-256b}$$

and

$$\begin{aligned} M(\overline{\sigma}'\overline{\mu}'\overline{\beta}'\overline{\nu}'\nu'', \sigma'\nu'\beta'\nu'\nu'') &= \sum_{\sigma''\mu''\beta''} C^{[\overline{\nu}']\beta',[\nu'']\beta''}_{\overline{\sigma}'\sigma'',\overline{\mu}'\mu''} C^{[\nu']\beta',[\nu'']\beta''}_{\sigma'\sigma'',\mu'\mu''} \\ &\times \begin{cases} \delta_{\overline{\mu}'\mu''} D^{[\sigma]}_{\overline{\sigma}'\sigma'',\sigma'\sigma''}(f_1 - 1, f_1), & \text{if } (f-1, f) \text{ is in } (\omega_1), \\ \delta_{\overline{\sigma}'\sigma''} D^{[\mu]}_{\overline{\mu}'\mu'',\mu'\mu''}(f_2 - 1, f_2), & \text{if } (f-1, f) \text{ is in } (\omega_2), \\ 1, \text{ if } (f-1, f) \text{ is not in the same } (\omega_i) \text{ and} \\ \quad \text{if } |\Psi^{\sigma}_{\overline{\sigma}'\sigma''} \Psi^{\mu}_{\overline{\mu}'\mu''}\rangle = (f-1, f) |\Psi^{\sigma}_{\sigma'\sigma''} \Psi^{\mu}_{\mu'\mu''}\rangle, \\ 0, \quad \text{otherwise}, \end{cases} \end{aligned} \tag{7-256c}$$

where σ'', μ'' and ν'' are the Young diagrams after deleting the index $f-1$ from the Young tableaux $\sigma' m'_1(\overline{\sigma}'\overline{m}'_1), \mu' m'_2(\overline{\mu}'\overline{m}'_2)$ and $\nu' m'$, respectively.

Equations (4-192) and (7-254) also provide a recursive approach to the calculation of the IDC. The degree of the eigenequation (4-192) satisfied by the $S_f \supset S_{f-1}$ outer-product ISF is much lower than the degree of (4-143) satisfied by the IDC of S_f. Therefore the recursive approach

to the IDC is more convenient than the direct approach. An efficient program was written for computing the outer-product ISF based on this algorithm (Novoselsky, [1] 1988).

Example 1: Find the $S_4 \supset S_3$ outer-product ISF $C^{[\nu][\nu']}_{\sigma\sigma',\mu\mu'}$ for $[\nu'] = [21], [\mu] = [1]$ and $[\sigma] = [21]$.

Step 1. According to the branching law, it is known that the possible values of $([\sigma'], [\mu'])$ are $([21], [0])$, $([2], [1])$ and $([11], [1])$. Since the $S_f \supset S_{f-1}$ outer-product ISF is independent of the component index m' in (7-252), we can set $m' = 1$. From (7-251) and Table 4.17-2 for the IDC of S_3, we can construct the following three basis vectors:

$$\begin{aligned}
\psi &= \left[\left|\begin{matrix}[21]\\[21]\end{matrix}\right\rangle \left|\begin{matrix}[1]\\[0]\end{matrix}\right\rangle\right]^{[21]}_1 = \left|\begin{matrix}\boxed{1}\boxed{2}\\\boxed{3}\end{matrix}, \boxed{4}\right\rangle = \psi_1 \ , \\
\psi_2 &= \left[\left|\begin{matrix}[21]\\[2]\end{matrix}\right\rangle \left|\begin{matrix}[1]\\[1]\end{matrix}\right\rangle\right]^{[21]}_1 = \sqrt{\frac{1}{6}}\left(\left|\begin{matrix}\boxed{1}\boxed{2}\\\boxed{4}\end{matrix}, \boxed{3}\right\rangle - \left|\begin{matrix}\boxed{1}\boxed{3}\\\boxed{4}\end{matrix}, \boxed{2}\right\rangle - \left|\begin{matrix}\boxed{2}\boxed{3}\\\boxed{4}\end{matrix}, \boxed{1}\right\rangle\right) \\
&= \sqrt{\tfrac{2}{3}}\psi_2 - \sqrt{\tfrac{1}{3}}\,\psi_3 \ , \\
\psi_3 &= \left[\left|\begin{matrix}[21]\\[11]\end{matrix}\right\rangle \left|\begin{matrix}[1]\\[1]\end{matrix}\right\rangle\right]^{[21]}_1 = \sqrt{\frac{1}{2}}\left(\left|\begin{matrix}\boxed{1}\boxed{4}\\\boxed{3}\end{matrix}, \boxed{2}\right\rangle + \left|\begin{matrix}\boxed{2}\boxed{4}\\\boxed{3}\end{matrix}, \boxed{1}\right\rangle\right) = \psi_4 \ ,
\end{aligned} \tag{7-257}$$

where $(\psi_1, \ldots, \psi_4)$ is the basis defined in (4-149b). From (4-149c) we obtain the matrix representative of the operator $C'(4) = C(4) - C(3)$ in the basis $(\psi_1, \ldots, \psi_4)$,

$$C'(4) = C^{(+)}(4) - C^{(+)}(3) = \begin{pmatrix} 0 & 1 & -\sqrt{\frac{1}{2}} & \sqrt{\frac{3}{2}} \\ 1 & -1 & 0 & 0 \\ -\sqrt{\frac{1}{2}} & 0 & -1 & 0 \\ \sqrt{\frac{3}{2}} & 0 & 0 & 1 \end{pmatrix} . \tag{7-258}$$

From (7-257) and (7-258) we find the matrix representative of $C'(4)$ in the basis $(\varphi_1, \varphi_2, \varphi_3)$,

$$M = \begin{pmatrix} 0 & \sqrt{\frac{3}{2}} & \sqrt{\frac{3}{2}} \\ \sqrt{\frac{3}{2}} & -1 & 0 \\ \sqrt{\frac{3}{2}} & 0 & 1 \end{pmatrix} . \tag{7-259}$$

A diagonalization of M yields the three eigenvalues 2, 0, -2, corresponding to the irreps $[\nu] = [31], [22], [211]$, and three eigenvectors, giving the $S_4 \supset S_3$ outer-product ISF listed in Table 7.17-2. This table is the same to within phase factors as Haacke's Table II for the $SU_4 \supset SU_3$ ISF.

Table 7.17-2. $S_4 \supset S_3$ outer-product ISF and $SU_n \supset SU_{n-1}$ ISF $C^{[\nu][\nu']}_{\sigma\sigma',\mu\mu'}$.

$\sigma'\sigma', \mu\mu'$ \ $[\nu']$ $[\nu]$	[31]	[21] [22]	[211]
[21][21], [1][0]	$\sqrt{3/8}$	1/2	$\sqrt{3/8}$
[21][11], [1][1]	3/4	$\sqrt{3/8}$	−1/4
[21][2], [1][1]	1/4	$-\sqrt{3/8}$	−3/4

7.17.2. The $S_f \supset S_{f_{12}} \otimes S_{f_{34}}$ outer-product ISF ($SU_f \supset SU_{f_{12}} \otimes SU_{f_{34}}$ ISF)

This subsection is analogous to Sec. 4.19.6. The notation for the particle numbers are the same as that given in (7-212a). Divide the number $1, 2, \ldots, f$ into four sets $(\omega_1'), (\omega_2'), (\omega_3')$ and (ω_4'), each of them being a normal order sequence:

$$(\omega_1') = (a_1, \ldots, a_{f_1}) \ , \quad (\omega_2') = (a_{f_1+1}, \ldots, a_{f_{12}}) \ , \tag{7-260}$$

$$(\omega_1'') = (a_{f_{12}+1}, \ldots, a_{f_{123}}) \ , \quad (\omega_2'') = (a_{f_{123}+1}, \ldots, a_f) \ ,$$

$$(\omega') = (\omega_1', \omega_2'), (\omega'') = (\omega_1'', \omega_2'') \ , \quad (\omega_1) = (\omega_1', \omega_1''), (\omega_2) = (\omega_2', \omega_2'') \ , \tag{7-261}$$

where (ω_1') and (ω_2') are the normal order sequences taken from $(1, 2, \ldots, f_{12})$ and (ω_1'') and (ω_2'') are those taken from $(f_{12}+1, \ldots, f)$ [see (4-129)]. The single particle states with the particle numbers $1, 2, \ldots, f_{12}$ and $f_{12}+1, \ldots f$ span the defining rep of $SU_{f_{12}}$ and $SU_{f_{34}}$, respectively. We shall use the following notation to denote the nine irreps of the three unitary groups along with the corresponding particle numbers and normal order sequences:

$$\begin{pmatrix} \sigma' & \mu' & \nu'_{\beta'} \\ \sigma'' & \mu'' & \nu''_{\beta''} \\ \sigma_\theta & \mu_\varphi & \nu_{\tau,\beta} \end{pmatrix} \begin{pmatrix} SU_{f_{12}} & SU_{f_{12}} & SU_{f_{12}} \\ SU_{f_{34}} & SU_{f_{34}} & SU_{f_{34}} \\ SU_f & SU_f & SU_f \end{pmatrix} \begin{pmatrix} f_1 & f_2 & f_{12} \\ f_3 & f_4 & f_{34} \\ f_{13} & f_{24} & f \end{pmatrix} \begin{pmatrix} \omega_1' & \omega_2' & \omega' \\ \omega_1'' & \omega_2'' & \omega'' \\ \omega_1 & \omega_2 & \omega \end{pmatrix} . \tag{7-262}$$

$$\begin{array}{llll} \beta' = 1, 2, \ldots \{\sigma'\mu'\nu'\} \ , & \beta'' = 1, 2, \ldots, \{\sigma''\mu''\nu''\} \ , & \beta = 1, 2, \ldots \{\sigma\mu\nu\} \ , \\ \theta = 1, 2, \ldots \{\sigma'\sigma''\sigma\} \ , & \varphi = 1, 2, \ldots \{\mu'\mu''\mu\} & \tau = 1, 2, \ldots \{\nu'\nu''\nu\} \end{array} .$$

For example $[\nu'']$ labels the irrep of $SU_{f_{34}}$ with f_{34} particles, and the irreducible basis of $SU_{f_{34}}$ and $S_{f_{34}}$ is $|Y^{(\nu'')}_{m''}(\omega'')\rangle = \left| \begin{matrix} [\nu''] \\ m''\omega'' \end{matrix} \right\rangle$.

We introduce the following three non-standard bases of the permutation groups $S_{f_{13}}, S_{f_{24}}$ and S_f:

$$\left| \begin{matrix} [\sigma] \\ \theta[\sigma']m_1'[\sigma'']m_1'' \end{matrix} \right\rangle, \left| \begin{matrix} [\mu] \\ \varphi[\mu']m_2'[\mu'']m_2'' \end{matrix} \right\rangle, \left| \begin{matrix} [\nu] \\ \tau[\nu']m'[\nu'']m'' \end{matrix} \right\rangle \tag{7-263}$$

$$S_{f_{13}} \supset S_{f_1} \otimes S_{f_3} \quad S_{f_{24}} \supset S_{f_2} \otimes S_{f_4} \quad S_f \supset S_{f_{12}} \otimes S_{f_{34}}.$$

They are also the $SU_f \supset SU_{f_{12}} \otimes SU_{f_{34}}$ irreducible bases. For example, $\left| [42], \begin{matrix} \boxed{1}\boxed{2}\boxed{4} \\ \boxed{3} \end{matrix} \ \boxed{5}\boxed{6} \right\rangle$ is the $SU_6 \supset SU_4 \otimes SU_2$ basis, belonging to the irreps [42], [31] and [2] of SU_6, SU_4 and SU_2, respectively.

The former two in (7-263) can be linearly combined into the third one through the following two steps:

1. Use the IDC of $S_{f_{12}}$ (the CGC of $SU_{f_{12}}$) and $S_{f_{34}}$ (the CGC of SU_{34}) to combine them into the standard basis $[\nu']m'$ of $S_{f_{12}}$ (the Gel'fand basis of $SU_{f_{12}}$) and $[\nu'']m''$ of $S_{f_{34}}$ (the Gel'fand basis of $SU_{f_{34}}$),

$$|(\sigma'\sigma'')_\theta(\mu'\mu'')_\varphi\beta\beta'\rangle \equiv \left[\left| \begin{matrix} [\sigma] \\ \theta[\sigma'][\sigma''] \end{matrix} \right\rangle \left| \begin{matrix} [\mu] \\ \varphi[\mu'][\mu''] \end{matrix} \right\rangle \right]^{[\nu']_{\beta'}[\nu'']_{\beta''}}_{m'm''}$$

$$= \sum_{m_1'm_2'\omega'm_1''m_2'',\omega''} C^{[\nu']\beta',m'}_{\sigma'm_1',\mu'm_2',\omega'} C^{[\nu'']\beta'',m''}_{\sigma''m_1'',\mu''m_2'',\omega''} \left| \begin{matrix} [\sigma] \\ \theta\sigma'm_1'\omega_1', \sigma''m_1''\omega_1'' \end{matrix} \right\rangle \left| \begin{matrix} [\mu] \\ \varphi\mu'm_2'\omega_2', \mu''m_2''\omega_2'' \end{matrix} \right\rangle . \tag{7-264}$$

2. Use the $S_f \supset S_{f_{12}} \otimes S_{f_{34}}$ outer-product ISF to combine (7-264) into the $S_f \supset S_{f_{12}} \otimes S_{f_{34}}$ irreducible basis (the $SU_f \supset SU_{f_{12}} \otimes SU_{f_{34}}$ basis)

$$\left| \begin{matrix} [\nu]\beta \\ \tau[\nu']m'[\nu'']m'' \end{matrix} \right\rangle = \sum_{\substack{\theta\sigma'\sigma''\beta' \\ \varphi\mu'\mu''\beta''}} C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\varphi\mu'\mu''} \left[\left| \begin{matrix} [\sigma] \\ \theta[\sigma'][\sigma''] \end{matrix} \right\rangle \left| \begin{matrix} [\mu] \\ \varphi[\mu'][\mu''] \end{matrix} \right\rangle \right]^{[\nu']_{\beta'}[\nu'']_{\beta''}}_{m'm''} . \tag{7-265}$$

which has the same form as (4-200) and an inverse expansion identical to (4-201).

7.17.3. The $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF and $S_f \supset S_{f_{12}} \otimes S_{f_{34}}$ outer-product ISF

In the above discussion, we only considered the permutation group and the unitary group in coordinate space. Now we want to take into account the unitary groups in state space which are designated by the script letter $\mathcal{U}$. We introduce the following symbols to denote the irreps of $\mathcal{SU}_m, \mathcal{SU}_n, \mathcal{SU}_{m+n}$ and the permutation groups:

$$\begin{pmatrix} \sigma' & \mu' & \nu'_{\beta'} \\ \sigma'' & \mu'' & \nu''_{\beta''} \\ \sigma_\theta & \mu_\varphi & \nu_{\tau,\beta} \end{pmatrix} , \quad \begin{pmatrix} \mathcal{SU}_m & \mathcal{SU}_n & \mathcal{SU}_{m+n} \\ \mathcal{SU}_m & \mathcal{SU}_n & \mathcal{SU}_{m+n} \\ \mathcal{SU}_m & \mathcal{SU}_n & \mathcal{SU}_{m+n} \end{pmatrix} , \quad \begin{pmatrix} f_1 & f_2 & f_{12} \\ f_3 & f_4 & f_{34} \\ f_{13} & f_{24} & f \end{pmatrix} . \tag{7-266}$$

Let

$$\left| \begin{matrix} [\nu'] \\ \beta'\sigma'w'_1\mu'w'_2 \end{matrix} \right\rangle , \quad \left| \begin{matrix} [\nu''] \\ \beta''\sigma''w''_1\mu''w''_2 \end{matrix} \right\rangle , \quad \left| \begin{matrix} [\nu] \\ \beta\sigma w_1\mu w_2 \end{matrix} \right\rangle \tag{7-267}$$

be the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ bases for particles $(1, 2, \ldots, f_{12}), (f_{12}+1, \ldots, f)$ and $(1, 2, \ldots, f)$, respectively. The $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF are defined by an expansion identical to (7-224). Equations (7-225)-(7-227) are still valid. Analogously, we can prove (Chen, Chen & Gao 1984) that the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF are precisely the $S_f \supset S_{f_{12}} \otimes S_{f_{34}}$ outer-product ISF, that is,

$$C^{[\nu]_\tau,\beta[\sigma]_\theta[\mu]_\varphi}_{\nu'\beta'\sigma'\mu',\nu''\beta''\sigma''\mu''} = C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{\sigma\theta\sigma'\sigma'',\mu\varphi\mu'\mu''} . \tag{7-268a}$$

$\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF $\quad S_f \supset S_{f_{12}} \otimes S_{f_{34}}$ outer-product ISF

Therefore the values of the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF do not depend explicitly on m and n, and all the remarks about the $\mathcal{SU}_{mn} \supset \mathcal{SU}_m \times \mathcal{SU}_n$ ISF apply to the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes SU_n$ ISF as well.

A special case of (7-268a) is

$$C^{[\nu],\beta\sigma\mu}_{\nu'\beta'\sigma'\mu',[1][1][0]} = C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'} . \tag{7-268b}$$

It shows that the $S_f \supset S_{f-1}$ outer-product ISF is the $SU_{mn} \supset SU_m \otimes SU_n$ one-body CFP, which gives the probability amplitude that the f particles are in the $SU_{mn} \supset SU_m \otimes SU_n$ state $|[\nu]\beta\sigma\mu\rangle$ after adding the last particle to the state $|[\nu']\beta'\sigma'\mu\rangle$.

A special case of the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF is the $\mathcal{SU}_n \supset \mathcal{SU}_{n-1} \otimes \mathcal{U}_1$ ISF, abbreviated to $\mathcal{SU}_n \supset \mathcal{SU}_{n-1}$ ISF, or called the $\mathcal{SU}_{n-1}$ *singlet factor*. For $\mathcal{SU}_n \supset \mathcal{SU}_{n-1} \times \mathcal{U}_1$ ISF, the irreps $[\mu'], [\mu'']$ and $[\mu]$ of the group $\mathcal{U}_1$ must be totally symmetric, that is, $[\mu'] = [f_2], [\mu''] = [f_4]$ and $[\mu] = [f_{24}]$, and (7-268) becomes

$$C^{[\nu]_\tau,[\sigma]_\theta[f_{24}]}_{[\nu'][\sigma'][f_2],[\nu'']][\sigma'']][f_4]} = C^{[\nu],\tau[\nu'][\nu'']}_{[\sigma]\theta[\sigma'][\sigma''],[f_{24}][f_2][f_4]} .$$

$\mathcal{SU}_{n-1}SF \qquad S_f \supset S_{f_{12}} \otimes S_{f_{34}}$ outer-product ISF $\tag{7-269}$

where we have dropped the redundant indices φ, β, β' and β''.

7.17.4. The evaluation of $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF

In analogy with the derivation of (7-236b), the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF can be expressed in terms of the IDC of $S_{f_{12}}, S_{f_{34}}$ and S_f, and the SDC of $S_{f_{13}}, S_{f_{24}}$ and S_f,

$$C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{[\nu']\beta'\sigma'\mu',\nu''\beta''\sigma''\mu''} = \sum_{m m_1 m_2 \omega m_1'' m_2''}^{\text{fix } m' m''} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2,\omega} C^{[\nu']\beta',m'}_{\sigma' m_1',\mu' m_2',\omega'} C^{[\nu'']\beta'',m''}_{\sigma'' m_1'',\mu'' m_2'',\omega''}$$
$$\times \left\langle \begin{matrix} [\nu] \\ m \end{matrix} \middle| [\nu], \begin{matrix} \tau\nu'\nu'' \\ m'm'' \end{matrix} \right\rangle \left\langle \begin{matrix} [\sigma] \\ m_1 \end{matrix} \middle| [\sigma] \begin{matrix} \theta\sigma'\sigma'' \\ m_1' m_1'' \end{matrix} \right\rangle \left\langle \begin{matrix} [\mu] \\ m_2 \end{matrix} \middle| [\mu], \begin{matrix} \varphi\mu'\mu'' \\ m_2' m_2'' \end{matrix} \right\rangle . \tag{7-270}$$

Noting that $(\omega_0) = (\omega_1, \omega_2)$, we know from (7-261) that the sum over ω implies a sum over ω' and ω''.

For the two-particle CFP, (7-270) can be further simplified

(a) $[\mu''] = [0]$,

$$C^{[\nu],\beta\sigma\mu}_{[\nu']\sigma'\mu',[\nu'']\sigma''][0]} = \delta_{\nu''\sigma''} \left(\langle [\nu] m | [\nu''] \rangle C^{[\nu']m'}_{\sigma' m_1',\mu' m_2',\omega'} \right)^{-1} \sum_{m_1}^{\text{fix } m_1'} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2,\omega} \langle [\sigma] m_1 | [\sigma''] \rangle . \tag{7-271a}$$

For $[\sigma''] = [0]$ we have a similar result.

(b) $[\sigma''] = [\mu''] = [1]$

$$C^{[\nu]\beta[\sigma][\mu]}_{[\nu']\sigma'\mu',[\nu'']1][1]} = (\langle [\nu] m | [\nu''] \rangle C^{[\nu']m'}_{\sigma' m_1',\mu' m_2',\omega'})^{-1} \sum_{m_1 m_2 \omega''}^{\text{fix } m_1' m_2' \omega'} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2,\omega} C^{[\nu'']}_{[1],[1],\omega''} . \tag{7-271b}$$

Example 2: Single-particle CFP. For the single-particle CFP, the expression (7-224b) can be written concisely as

$$\left| \begin{matrix} [\nu] \\ \beta\sigma\mu \end{matrix} \right\rangle = \sum_{\beta'\sigma'} C^{[\nu],\beta\sigma\mu}_{\nu'\beta'\sigma'\mu,[1][1][0]} \left| \begin{matrix} [\nu'] \\ \beta'\sigma'\mu \end{matrix} \right\rangle |\psi(f)\rangle + \sum_{\beta'\mu'} C^{[\nu],\beta\sigma\mu}_{\nu'\beta'\sigma\mu',[1][0][1]} \left| \begin{matrix} [\nu'] \\ \beta'\sigma\mu' \end{matrix} \right\rangle |\varphi(f)\rangle , \tag{7-272}$$

where $\psi(f)$ belongs to the defining rep [1] of $\mathcal{SU}_m$ and $\varphi(f)$ belongs to that of $\mathcal{SU}_n$.

From the IDC tables, Table 4.17-5d, and Table 8f(1) (Chen & Gao 1981), and using (7-254b) we obtain

$$\left| \begin{matrix} [321] \\ \alpha[21][21] \end{matrix} \right\rangle = \sqrt{\frac{9}{20}} \left(\left| \begin{matrix} [32] \\ [2][21] \end{matrix} \right\rangle |\psi(6)\rangle + \left| \begin{matrix} [32] \\ [21][2] \end{matrix} \right\rangle |\varphi(6)\rangle \right)$$
$$+ \sqrt{\frac{1}{20}} \left(\left| \begin{matrix} [32] \\ [11][21] \end{matrix} \right\rangle |\psi(6)\rangle + \left| \begin{matrix} [32] \\ [21][11] \end{matrix} \right\rangle |\varphi(6)\rangle \right) .$$

$$\left| \begin{matrix} [321] \\ \beta[21][21] \end{matrix} \right\rangle = \frac{1}{2} \left(- \left| \begin{matrix} [32] \\ [2][21] \end{matrix} \right\rangle |\psi(6)\rangle + \left| \begin{matrix} [32] \\ [21][2] \end{matrix} \right\rangle |\varphi(6)\rangle \right.$$
$$\left. + \left| \begin{matrix} [32] \\ [11][21] \end{matrix} \right\rangle |\psi(6)\rangle - \left| \begin{matrix} [32] \\ [21][11] \end{matrix} \right\rangle |\psi(6)\rangle \right) .$$

7.17.5. Symmetries of the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF

The symmetries (7-239) and (7-240) still hold for the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF, with the exception that $H_\nu(SU_{mn})$ and $H_{\nu'}(SU_{mn})$ should be replaced by $H_\nu(SU_{m+n})$ and $H_{\nu'}(SU_{m+n})$.

Due to (7-268b), (7-254b) and (4-153c), in case of $\{\sigma\mu\nu\} = 1$, the one-body ISF has the symmetry

$$C^{[\nu],\beta\sigma\mu}_{\nu'\beta'\sigma'\mu',[1][1][0]} = (-1)^{[\sigma]+[\mu]+[\nu]+[\sigma']+[\mu']+[\nu']} C^{[\nu],\beta\mu\sigma}_{\nu'\beta'\mu'\sigma',[1][0][1]} \,. \tag{7-273a}$$

For example, for $\mathcal{SU}_4 \supset \mathcal{SU}_2 \otimes \mathcal{SU}_2$ ISF, the symmetries (7-239b) and (7-240) tell us that

$$\begin{aligned} C^{[321][21][21]}_{[31][11][2],[11][1][1]} &= \varepsilon_2 C^{[4321][32][32]}_{[332][22][31],[11][1][1]} \\ &= \varepsilon_3 \left(\sqrt{\frac{1\times 3}{H_{[332]}(SU_4)}} \Big/ \sqrt{\frac{2\times 2}{H_{[321]}(SU_4)}} \right) C^{[332][22][31]}_{[321][21][21],[11][1][1]} \,. \end{aligned}$$

If the first coefficient is regarded as the $\mathcal{SU}_5 \supset \mathcal{SU}_3 \otimes \mathcal{SU}_2$ ISF, we have

$$\begin{aligned} C^{[321][21][21]}_{[31][11][2],[11][1][1]} &= \varepsilon_2 C^{[4^2321][432][32]}_{[3^32][32^2][31],[1^3][11][1]} \\ &= \varepsilon_3 \left(\sqrt{\frac{3\times 3}{H_{[3^32]}(SU_5)}} \Big/ \sqrt{\frac{2\times 8}{H_{[321]}(SU_5)}} \right) C^{[3^32][322][31]}_{[3321][321][21],[11][1][1]} \,. \end{aligned}$$

In addition, the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF also have the following symmetries:

1. From (7-269a) we know that the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF is invariant under the interchange of indices,

$$\mu' \leftrightarrow \sigma'' \,, \quad \nu' \leftrightarrow \sigma \,, \quad \nu'' \leftrightarrow \mu \,, \quad \beta \leftrightarrow \tau \,, \quad \beta' \leftrightarrow \theta \,, \quad \beta'' \leftrightarrow \varphi \,,$$

which can also be written as

$$\begin{pmatrix} \sigma' & \mu' & \nu'_{\beta'} \\ \sigma'' & \mu'' & \nu''_{\beta''} \\ \sigma_\theta & \mu_\varphi & \nu_{\tau,\beta} \end{pmatrix} \leftrightarrow \begin{pmatrix} \sigma' & \sigma'' & \sigma_\theta \\ \mu' & \mu'' & \mu_\varphi \\ \nu'_{\beta'} & \nu''_{\beta''} & \nu_{\beta,\tau} \end{pmatrix} \,. \tag{7-273b}$$

2. By using the symmetry of the IDC, (4-162a), and the symmetry of the SDC, Eq. (4-180a), one gets from (7-270)

$$C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\varphi}_{\nu'\beta'\sigma'\mu',\nu''\beta''\sigma''\mu''} = \varepsilon C^{[\tilde\nu]\tau,\beta[\tilde\sigma]\theta[\tilde\mu]\varphi}_{\tilde\nu'\beta'\tilde\sigma'\tilde\mu,\tilde\nu''\beta''\tilde\sigma''\tilde\mu''} \,, \tag{7-273c}$$

where ε is a phase factor depending on the phase convention.

The relation between the $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ ISF and the 9ν coefficients of $\mathcal{SU}_{m+n}$ is given in (9-26).

The single-particle CFP for $\mathcal{SU}_{m+n} \supset \mathcal{SU}_m \otimes \mathcal{SU}_n$ have been tabulated for systems with up to six particles (Chen, Chen & Gao 1984), and to twelve particles (Vallieres & Novoselsky 1994).

7.18. The SU_n Singlet Factor

Since the $SU_{m+n} \supset SU_m \otimes SU_n$ ISF do not depend on m and n explicitly, the SU_n SF (singlet factor) also do not depend on n explicitly. Therefore any given SU_n SF gives an infinite number of SU_m SF,

$$(SU_m\text{SF}) = (SU_n\text{SF}) \,, \quad m = n+1, n+2, \ldots \,. \tag{7-274a}$$

Of course, not every SU_n SF can be deduced from the SU_{n-1} SF. We call an SU_n SF derivable, if it can be deduced from the SU_{n-1} SF through the equation SU_n SF $= SU_{n-1}$ SF, otherwise we call it underivable. It is very simple to see whether an SU_n SF $C^{[\nu]\tau,[\sigma]\theta[f_{24}]}_{[\nu'][\sigma'][f_2],[\nu'']][\sigma'']][f_4]}$ is derivable or not. If the Young diagram $[\sigma]$ has r rows, then the SU_r SF is underivable, and the SU_n SF with $n > r$ is derivable, that is,

$$(SU_n \text{ SF}) = (SU_r \text{ SF}) \,, \quad \text{for } n = r+1, r+2, \ldots \,. \tag{7-274b}$$

Equations (7-147) and (7-274) show that the calculation of the SU_n CG coefficients in the Gel'fand basis is reduced to the calculation of a few underivable SU_r SF, which can be obtained from (7-270).

That the SU_n SF are independent of n escaped our attention for many years. The reason for this oversight is that we generally use specific quantum numbers for specific n, rather than the partitions, to label the irreps of SU_n. Table 7.18-1 gives the labelling schemes which are in common use.

Table 7.18-1. The usual labelling schemes for irreps $[\nu]$, $[\sigma]$ and $[\mu]$.

	$[\nu]$	$[\sigma]$	$[\mu]$
SU_2 CGC	isospin I		$I_z = \frac{1}{2}(n_1 - n_2)$[1)]
$SU_3 \supset SU_2 \otimes U_1$ ISF	$(\lambda\mu)$ or dim. of SU_3	$2I+1$	$Y = \frac{1}{3}(n_1 + n_2 - 2n_3)$
$SU_4 \supset SU_3 \otimes U_1$ ISF	dim. of SU_4	dim. of SU_3	$Z = \frac{1}{4}(n_1 + n_2 + n_3 - 3n_4)$

[1)] Here $[\sigma] = [n_1]$, $[\mu] = [n_2]$.

In the past, the calculation and tabulation of the SU_n SF were done for one n at a time. With the discovery of the relation (7-274), and using the partitions as labels, we can revolutionalize the tabulation of the SU_n SF, so that from a given table we can read out an infinite number of SU_n SF of the same type. Tables 7.18-2 and 7.18-3 are two examples of such tabulations. From them one can read out all the SU_n SF of the same type with $n = r, r+1, r+2\ldots$, where r is the number of rows of the blank Young diagram $[\sigma]$ (without being filled with the letter n) in the table headings. For example, Table 7.18-2 covers the SU_2 CGC table (Rotenberg 1959), the SU_2 SF table (de Swart 1963), and the SU_3 SF table (Haacke 1976), and Table 7.18-3 covers the SU_2 SF and SU_3 SF table.

7.19. Second Quantized Expressions for the CFP

The total CFP can be written in second quantized form, which is quite useful. We use the round brackets, $(\ |$, or $|\ )$, to denote a second quantized state, while the ordinary bracket, $\langle\ |$, or $|\ \rangle$, an ordinary quantized state. The following discussions are valid both for fermions and bosons.

7.19.1. One-particle CFP

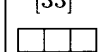
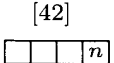
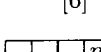
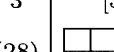
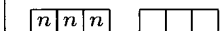
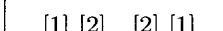
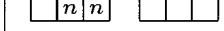
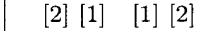
Suppose that we have n identical fermions in a state $|[1^n]\alpha JM)$ which is an $SU_n \supset SO_3$ irreducible basis, α being additional quantum numbers which may be the irrep labels of another group (or groups) inserted between SU_N and SO_3. Let $b^\dagger_{jm}$ and b_{jm} be creation and annihilation operators. Applying the number operator $\hat{n} = \sum_{jm} b^\dagger_{jm} b_{jm}$ to the state $|[1^n]\alpha JM)$, we have

$$n|[1^n]\alpha JM) = \sum_{jm} C^\dagger_{jm} C_{jm} |[1^n]\alpha JM) \ . \tag{7-275}$$

Inserting a unit operator between $C^\dagger_{jm}$ and C_{jm}, we find

$$\begin{aligned} n|[1^n]\alpha JM) &= \sum_{\alpha_1 J_1 M_1 jm} C^\dagger_{jm} |[1^{n-1}]\alpha_1 J_1 M_1) \big([1^{n-1}]\alpha_1 J_1 M_1 | C_{jm} |[1^n]\alpha JM\big) \\ &= \sum_{\alpha_1 J_1 M_1 jm} C^\dagger_{jm} |[1^{n-1}]\alpha_1 J_1 M_1) \big([1^n]\alpha JM | C^\dagger_{jm} |[1^{n-1}]\alpha_1 J_1 M_1\big) \\ &= \sum_{\alpha_1 J_1 j} (-1)^{J_1 + j - J} \left[C^\dagger_j |[1^{n-1}]\alpha_1 J_1)\right]^J_M \big([1^n]\alpha J \big\| C^\dagger_j \big\| [1^{n-1}]\alpha_1 J_1\big) \ . \end{aligned} \tag{7-276}$$

Table 7.18-2 $SU_n \supset SU_{n-1} \otimes U_1$ ISF $C^{[\nu],[3][3]}_{[3][\sigma'][\mu'],[3][\sigma''][\mu'']}$

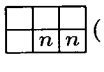
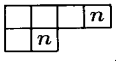
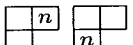
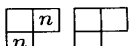
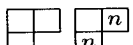
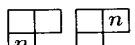
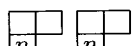
(SU_2 CGC) / 0	(SU_2 SF) / $4, -1$	(SU_3 SF) / $(10), -\frac{3}{2}$	$[\sigma']\ [\mu']$ $[\sigma'']\ [\mu'']$	[33] 0  (10*) 50	[42] 1  (27) 126	[6] 3  (28) 84″	[51] 2  (35) 140
$\frac{3}{2} - \frac{3}{2}, \frac{3}{2}\frac{3}{2}$	$1, -2; 4, 1$	$(1) - \frac{9}{4}, (10)\frac{3}{4}$	[0] [3] [3] [0] 	$-\frac{1}{2}$	$\frac{3}{2\sqrt{5}}$	$\frac{1}{2\sqrt{5}}$	$-\frac{1}{2}$
$\frac{3}{2} - \frac{1}{2}, \frac{3}{2}\frac{1}{2}$	$2, -1; 3, 0$	$(3) - \frac{5}{4}, (6) - \frac{1}{4}$	[1] [2] [2] [1] 	$\frac{1}{2}$	$-\frac{1}{2\sqrt{5}}$	$\frac{3}{2\sqrt{5}}$	$-\frac{1}{2}$
$\frac{3}{2}\frac{1}{2}, \frac{3}{2} - \frac{1}{2}$	$3, 0; 2, -1$	$(6) - \frac{1}{4}, (3) - \frac{5}{4}$	[2] [1] [1] [2] 	$-\frac{1}{2}$	$-\frac{1}{2\sqrt{5}}$	$\frac{3}{2\sqrt{5}}$	$\frac{1}{2}$
$\frac{3}{2}\frac{3}{2}, \frac{3}{2} - \frac{3}{2}$	$4, 1; 1, -2$	$(10)\frac{3}{4}, (10) - \frac{9}{4}$	[3] [0] [0] [3] 	$\frac{1}{2}$	$\frac{3}{2\sqrt{5}}$	$\frac{1}{2\sqrt{5}}$	$\frac{1}{2}$

The meaning of the table heading is

SU_1 SF (SU_2 CGC) I_z	(SU_2 SF) λ, Y	(SU_3 SF) $(h_\sigma)Z$	$\begin{pmatrix}[\nu]\\[\sigma][\mu]\end{pmatrix}$ / $\begin{pmatrix}[\nu']\\[\sigma'][\mu']\end{pmatrix}\begin{pmatrix}[\nu'']\\[\sigma''][\mu'']\end{pmatrix}$	diagram I (h_ν) $\underline{H}_\nu$	SU_1 SF SU_2 SF SU_3 SF
$I'I'_zI''I''_z$	$\lambda'Y', \lambda''Y''$	$(h_{\sigma'})Z', (h_{\sigma''})Z''$	diagram (entries)		

1) Where the irreps of SU_2, SU_3 and SU_4 are labelled by $2I+1$, $\dim(h)$, and $\dim(H)$, respectively (for dimension tables, see Table A1 in the Appendix).
2) The total Young diagram and the one formed by the blank boxes are the irrep labels of SU_n and SU_{n-1} respectively.

Table 7.18-3 $SU_n \supset SU_{n-1} \otimes U_1$ ISF $C^{[\nu]\tau,[31][2]}_{[21][\sigma'][\mu'],[21][\sigma''][\mu'']}$, $\tau = D, F$

(SU_2 SF)	(SU_3 SF)		$[\sigma'][\mu'], [\sigma''][\mu'']$	$[321]D$  $(8D)$ $\underline{64D}$	$[321]D$  $(8F)$ $\underline{64F}$	$[411]$  (10) $\underline{70}$	$[33]$  (10^*) $\underline{50}$	$[42]$  (27) $\underline{1260}$
λ, Y $3, 0$	$(h_\sigma), Z$ $(15), -\frac{1}{2}$							
$\lambda'Y, \lambda''Y''$ $1,0;3,0$	$(h_{\sigma'})Z', (h_{\sigma''})Z''$ $(3^*) - \frac{1}{4}, (6) - \frac{1}{4}$		$[11][1], [2][1]$	$\frac{1}{\sqrt{5}}$	0	$-\frac{1}{2}$	$-\frac{1}{2}$	$\sqrt{\frac{3}{10}}$
$2, -1; 2, 1$	$(3) - \frac{5}{4}, (8)\frac{3}{4}$		$[1][2], [21][0]$	$-\sqrt{\frac{3}{10}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{5}}$
$2, 1; 2, -1$	$(8)\frac{3}{4}, (3) - \frac{5}{4}$		$[21][0], [1][2]$	$-\sqrt{\frac{3}{10}}$	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{5}}$
$3, 0; 1, 0$	$(6) - \frac{1}{4}, (3^*) - \frac{1}{4}$		$[2][1], [11][1]$	$\frac{1}{\sqrt{5}}$	0	$\frac{1}{2}$	$\frac{1}{2}$	$\sqrt{\frac{3}{10}}$
$3, 0; 3, 0$	$(6) - \frac{1}{4}, (6) - \frac{1}{4}$		$[2][1], [2][1]$	0	$\sqrt{\frac{2}{3}}$	$-\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	0

Multiplying (7-276) from the left with $\big([1^n]\alpha JM\big|$, we obtain

$$n = \sum_{\alpha_1 J_1 j} \big([1^n]\alpha J \parallel C_j^\dagger \parallel [1^{n-1}]\alpha_1 J_1\big)^2 . \tag{7-277}$$

The total anti-symmetric state can be expanded using the one–particle CFP,

$$|[1^n]\alpha JM\rangle = \sum_{\alpha_1 J_1 j} \langle [1^n]\alpha J|\{[1^{n-1}]\alpha_1 J_1, j\rangle \Big[\big|[1^{n-1}]\alpha_1 J_1\big\rangle\ \psi_j(n)\Big]^J_M , \tag{7-278}$$

Comparing (7-276) with (7-278), we see that the reduced matrix element is proportional to the CFP,

$$\big([1^n]\alpha J \parallel C_j^\dagger \parallel [1^{n-1}]\alpha_1 J_1\big) = \text{const}\,\langle [1^n]\alpha J\{|[1^{n-1}]\alpha_1 J_1, j\rangle . \tag{7-279}$$

From (7-277), (7-279) and the normalization of the CFP, we obtain const $= \sqrt{n}$. Thus

$$\big([1^n]\alpha J \parallel C_j^\dagger \parallel [1^{n-1}]\alpha_1 J_1\big) = \binom{n}{1}^{1/2} \langle [1^n]\alpha J\{|[1^{n-1}]\alpha_1 J_1, j\rangle . \tag{7-280}$$

The physical implication of (7-280) is clear; it says that the probability of separating *any one fermion* from an n–fermion anti–symmetric state is equal to n times the probability of separating *the n-th fermion* from the same state.

7.19.2. Two-particle CFP

It is easy to verify that for both fermions and bosons, we have the identity

$$\sum_{j_1, m_1 j_2 m_2} C^\dagger_{j_1 m_1} C^\dagger_{j_2 m_2} C_{j_2 m_2} C_{j_1 m_1} = \hat{n}^2 - \hat{n} . \tag{7-281}$$

Applying this to the state $|[1^n]\alpha JM)$, we get

$$\begin{aligned} n(n-1)|[1^n]\alpha JM) = & \sum_{j_1 m_1 j_2 m_2 \alpha_1 J_1 M_1} C^\dagger_{j_1 m_1} C^\dagger_{j_2 m_2} |[1^{n-2}]\alpha_1 J_1 M_1) \\ & \times \big([1^{n-2}]\alpha_1 J_1 M_1 | C_{j_2 m_2} C_{j_1 m_1} \big| [1^n]\alpha JM\big) . \end{aligned} \tag{7-282}$$

Using the relation

$$\sum_{j_1 j_2} = \frac{2}{1+\delta_{j_1 j_2}} \sum_{j_1 \le J_2} , \tag{7-283}$$

and the normalized pair creation operator

$$\mathcal{A}^\dagger(j_1 j_2 J_2 M_2) = \frac{1}{\sqrt{1+\delta_{j_1 j_2}}} [C^\dagger_{j_1} C^\dagger_{j_2}]^{J_2}_{M_2} , \tag{7-284}$$

Equation (7-282) can be written as

$$\begin{aligned} n(n-1)|[1^n]\alpha JM) = & \, 2 \sum_{j_1 \le j_2} \sum_{\alpha J_1 J_2} (-1)^{J_1 + J_2 - J} \Big[\mathcal{A}^\dagger(j_1 j_2 J_2)\Big|[1^{n-2}]\alpha_1 J_1\Big)\Big]^J_M \\ & \times \Big([1^n]\alpha J \parallel \mathcal{A}^\dagger(j_1 j_2 J_2) \parallel [1^{n-2}]\alpha_1 J_1\Big) . \end{aligned} \tag{7-285}$$

Therefore

$$\frac{n(n-1)}{2} = \sum_{j_1 \le j_2} \sum_{\alpha J_1 J_2} \big([1^n]\alpha J \parallel \mathcal{A}^\dagger(j_1 j_2 J_2) \parallel [1^{n-2}]\alpha_1 J_1\big)^2 . \tag{7-286}$$

On the other hand, from the expansion in terms of the CFP we have

$$|[1^n]\alpha JM\rangle = \sum_{j_1\le j_2,\alpha J_1 J_2} \langle [1^n]\alpha J_2\{|[1^{n-2}]\alpha_1 J_1\ , [1^2](j_1 j_2)J_2\rangle \Big[|[1^{n-2}]\alpha_1 J_1\rangle |[1^2](j_1 j_2)J_2\rangle\Big]^J_M\ , \tag{7-287}$$

where the sum is restricted to $j_1 \le j_2$, otherwise the states on the right-hand side of (7-287) would be overcomplete. Comparing (7-285) with (7-287), we know that

$$\big([1^n]\alpha J \parallel \mathcal{A}^\dagger(j_1 j_2 J_2) \parallel [1^{n-2}]\alpha_1 J_1\big) = \text{const}\,\langle [1^n]\alpha J\{|[1^{n-2}]\alpha_1 J_1, [1^2](j_1 j_2)J_2\rangle\ . \tag{7-288}$$

From (7-286) and (7-288) and the normalization of CFP, it follows that

$$\sum_{j_1\le j_2,\alpha J_1 J_2} \langle [1^n]\alpha J\{|[1^{n-2}]\alpha_1 J_1, [1^2](j_1 j_2)J_2\rangle^2 = 1\ , \tag{7-289}$$

and we finally get the required relation

$$\big([1^n]\alpha J \parallel \mathcal{A}^\dagger(j_1 j_2 J_2) \parallel [1^{n-2}]\alpha_1 J_1\big) = \binom{n}{2}^{1/2} \langle [1^n]\alpha J\{|[1^{n-2}]\alpha_1 J_1, [1^2](j_1 j_2)J_2\rangle\ . \tag{7-290}$$

The physical implication of (7-290) is again very clear.

7.19.3 CFP in the interacting boson model

In the interacting boson model (IBM) of nuclei (Arima 1981 and Sec. 9.10), there are two kinds of bosons $C^\dagger_l$ with $l = 0, 2$, which carry the defining rep of SU_6 and belong to the irrep (20) of SU_3. The two-boson state in the $SU_6 \supset SU_3 \supset SO_3$ group chain can be expressed as

$$|[2](\lambda_2\mu_2)L_2 M_2) = \mathcal{A}^\dagger((\lambda_2\mu_2)L_2 M_2)|0)\ ,$$

$$\mathcal{A}^\dagger((\lambda_2\mu_2)L_2 M_2) = \sum_{l_1\le l_2} C^{(\lambda_2\mu_2)L_2}_{(20)l_1,(20)l_2} \mathcal{A}^\dagger(l_1 l_2 L_2 M_2)\ . \tag{7-291a}$$

The first factor on the right-hand side is the $SU_3 \supset SO_3$ ISF. According to Elliott (1958), the permissible values of $(\lambda_2\mu_2)L_2$ are $(40)S, D, G$ and $(02)S, D$. The inverse of (7-291a) is

$$\mathcal{A}^\dagger(l_1 l_2 L_2 M_2) = \sum_{\lambda_2\mu_2} C^{(\lambda_2\mu_2)L_2}_{(20)l_1,(20)l_2} \mathcal{A}^\dagger((\lambda_2\mu_2)L_2 M_2)\ . \tag{7-291b}$$

For one-particle CFP we have

$$\Big([n](\lambda\mu)L \parallel C^\dagger_l \parallel [n-1](\lambda_1\mu_1)L_1\Big) = \binom{n}{1}^{1/2} C^{[n],(\lambda\mu)L}_{[n-1](\lambda_1\mu_1)L_1,[1](20)l}\ . \tag{7-292}$$

For two-particle CFP, we need a relation similar to (7-285), that is,

$$\begin{aligned} n(n-1)\big|[n](\lambda\mu)LM\big) = 2 \sum_{l_1\le l_2} \sum_{(\lambda_1\mu_1)L_1 L_2} (-1)^{L_1+L_2-L} \Big[\mathcal{A}^\dagger(l_1 l_2 L_2)\big|[n-2](\lambda_1\mu_1)L_1\big)\Big]^L_M \\ \times \Big([n](\lambda\mu)L \parallel \mathcal{A}^\dagger(l_1 l_2 L_2) \parallel [n-2](\lambda_1\mu_1)L_1\Big)\ . \end{aligned} \tag{7-293}$$

By using (7-291), (7-293) becomes

$$\begin{aligned} n(n-1)\big|[n](\lambda\mu)LM\big) = 2 \sum_{(\lambda_1\mu_1)L_1(\lambda_2\mu_2)L_2} (-1)^{L_1+L_2-L} \Big[\mathcal{A}^\dagger((\lambda_2\mu_2)L_2)\big|[n-2](\lambda_1\mu_1)L_1\big)\Big]^L_M \\ \times \Big([n](\lambda\mu)L \parallel \mathcal{A}^\dagger((\lambda_2\mu_2)L_2) \parallel [n-2](\lambda_1\mu_1)L_1\Big)\ . \end{aligned} \tag{7-294}$$

Therefore

$$\frac{n(n-1)}{2} = \sum_{(\lambda_1\mu_1)L_1(\lambda_2\mu_2)L_2} \Big([n](\lambda\mu)L \parallel \mathcal{A}^\dagger((\lambda_2\mu_2)L_2) \parallel [n-2](\lambda_1\mu_1)L_1\Big)^2 . \tag{7-295}$$

Thus the second quantized form of the two–particle CFP in the IBM is

$$\Big([n](\lambda\mu)L \parallel \mathcal{A}^\dagger((\lambda_2\mu_2)L_2) \parallel [n-2](\lambda_1\mu_1)L_1\Big) = \binom{n}{2}^{1/2} C^{[n](\lambda\mu)L}_{[n-2](\lambda_1\mu_1)L_1,[2](\lambda_2\mu_2)L_2} . \tag{7-296}$$

The extension of (7-292) and (7-296) to other group chains is trivial.

7.20. The Generalized Quantized Expressions for the CFP

7.20.1 The generalized quantization

We introduced the CFP for partial space (orbital, spin, or spin–isospin) using the first quantization in Sec. 7.13.2, and gave the second quantized expression for the total CFP in Sec. 7.19. The latter expression is more concise than the former. However the second quantization is applicable only to the totally symmetric or totally anti–symmetric states, the CFP in partial space cannot be expressed in the second quantized form. In this section we are going to show that by introducing a so–called *generalized quantization* formalism (Chen 1991), the expression of the partial CFP can be as concise as the total CFP in the second quantization. The generalized quantization formalism is in between the first and second quantizations, and contains the latter as its special case.

Suppose that in a certain space, which could be a partial space or a total space, we have a set of single–particle states $\alpha, \beta, \gamma \ldots$, which carry the fundamental representation of the unitary group SU_M.

Definition 7.1: The creation (annihilation) operator $a^\dagger_\alpha$ (a_α) in the generalized quantization formalism creates (annihilates) the *last* particle in the state α,

$$\begin{aligned} a^\dagger_\alpha|\Psi(1,2,\ldots,n-1)\rangle &= |\Psi(1,2,\ldots,n-1)\psi_\alpha(n)\rangle , \\ a_\alpha|\Psi(1,2,\ldots,n-1)\psi_\beta(n)\rangle &= \delta_{\alpha\beta}|\Psi(1,2,\ldots,n-1)\rangle . \end{aligned} \tag{7-297}$$

To examine the commutator relations of the hybrid operators, we use Definition 7.1 to get

$$\begin{aligned} a^\dagger_\alpha a^\dagger_\beta|\Psi(1,2,\ldots,n-2)\rangle &= |\Psi(1,2,\ldots,n-2)\psi_\beta(n-1)\psi_\alpha(n)\rangle, \\ a^\dagger_\beta a^\dagger_\alpha|\Psi(1,2,\ldots,n-2)\rangle &= |\Psi(1,2,\ldots,n-2)\psi_\alpha(n-1)\rangle\psi_\beta(n)\rangle . \end{aligned} \tag{7-298}$$

Therefore $a^\dagger_\alpha$ and $a^\dagger_\beta$ neither commute nor anti–commute. From Definition 7.1 it is obvious that

$$a_\alpha a^\dagger_\beta \equiv \delta_{\alpha\beta} .$$

Since the hybrid operators $a^\dagger_\alpha$ ($a^\dagger_\beta$) are the creation (annihilation) operators for a specific (the last) particle, they are factorizable,

$$a^\dagger_{jmtm'} = a^\dagger_{jm} a^\dagger_{tm'} . \tag{7-299}$$

This factorization is recursive and can be applied to any combined space. For example,

$$a^\dagger_{lcfs} = a^\dagger_l a^\dagger_{cfs} = a^\dagger_l a^\dagger_c a^\dagger_{fs} = a^\dagger_l a^\dagger_c a^\dagger_f a^\dagger_f ,$$

where l, c, f, s represent the orbital, color, flavor, and spin space, respectively. Obviously the hybrid operators acting on different subspaces commute.

As will be seen in Sec. 9.1 and 9.2, the factorizability of the hybrid operator has great significance in simplifying the calculation of the matrix elements of one– and two–body operators in a many–body system. It is noted that the operators in the second quantization formalism do not have such a factorization property.

7.20.2 The CFP in the generalized quantization

For the sake of convenience, we call $a^\dagger_\alpha$ (a_α) hybrid operators and use $\nu^{00}, \nu^0, \nu, \nu'$ and ν'' to denote the SU_M irrep labels for systems with $n+2, n+1, n, n-1$ and $n-2$ particles, respectively. Note that due to the branching law (see Sec. 4.3) for the permutation group we have

$$[\nu]m = [\nu][\nu']m' = [\nu][\nu'][\nu'']m'' \dots \ .$$

It is understood that in the following the partitions $[\nu^{00}], [\nu^0], [\nu], [\nu']$ and $[\nu'']$ have to obey the branching rule for Young diagrams.

In the partial space with first quantization we have to use two sets of quantum numbers, $[\nu]m$ and $[\nu]w$ (see (7-76)), referring to permutation group and unitary group respectively, to uniquely specify a basis vector $|[\nu]m, w> \equiv \left|\begin{smallmatrix}[\nu]\\ m,w\end{smallmatrix}\right\rangle$, where m is the index of the Yamanouchi symbol and w any convenient subgroup labels of the unitary group.

Applying $a^\dagger_\alpha$ to $|[\nu']m'w'\rangle$ and inserting the identity operator,

$$1 = \sum_{\nu m w} |[\nu]m, w\rangle\langle[\nu]m, w| \ , \tag{7-300a}$$

between the creation operator and state, we get

$$a^\dagger_\alpha|[\nu']m', w'\rangle = |[\nu']m', w'\rangle|\psi_\alpha(n)\rangle = \sum_{\nu m w} |[\nu]m, w\rangle n\langle[\nu]m, w|a^\dagger_\alpha|[\nu']m', w'\rangle \ . \tag{7-301}$$

Since $a^\dagger_\alpha$ is the creation operator for the the nth–particle, it is a scalar of S_{n-1}, and the matrix element $\langle[\nu]m, w|a^\dagger_\alpha|[\nu']m', w'\rangle$ is diagonal in m' and depends only on the quantum number $[\nu], w, [\nu']$ and w'. Therefore the matrix element of $a^\dagger_\alpha$ in (7-301) can be rewritten as

$$\langle[\nu]m, w|a^\dagger_\alpha|[\nu']m', w'\rangle = \langle[\nu]w|a^\dagger_\alpha|[\nu']w'\rangle \ , \tag{7-302}$$

while Eq. (7-301) can be simplified to

$$a^\dagger_\alpha|[\nu']w'\rangle = \sum_{\nu w} |[\nu]w\rangle\langle[\nu]w|a^\dagger_\alpha|[\nu']w'\rangle \ . \tag{7-303}$$

This shows that in the generalized quantization formalism, the indices for the permutation group can be ignored and the completeness condition (7-300a) reduces to

$$1 = \sum_{\nu w} |[\nu]w\rangle\langle[\nu]w| \ . \tag{7-300b}$$

The elimination of the permutation group labels is one of the advantages of the generalized quantization.

From (7-303) we know that the matrix element of the hybrid creation operator is just the CG coefficient of SU_M,

$$\langle[\nu]w|a^\dagger_\alpha|[\nu']w'\rangle = C^{[\nu]w}_{[\nu']w',[1]\alpha} \ . \tag{7-304}$$

Suppose that $|[\nu]\theta\Lambda m\rangle$ is the $SU_M \supset G \supset G(s)$ symmetry adapted basis, where θ is the inner multiplicity label for the subduction $SU_M \downarrow G$. From (7-304) and (3-302) we obtain the important conclusion that the G–reduced matrix element of $a^\dagger_\alpha$ is just the $SU_M \supset G$ ISF, or the $SU_M \supset G$ one–body CFP,

$$\langle [\nu]\theta\Lambda \parallel a^\dagger_\lambda \parallel [\nu']\theta'\Lambda'\rangle = C^{[\nu]\theta\Lambda}_{[\nu']\theta'\Lambda',[1]\lambda} \,. \tag{7-305}$$

The one–body CFP in (7-160) can be expressed as

$$\langle l^{n-1}[\nu_1]\alpha_1 L_1, l\}l^n[\nu]\alpha L\rangle = \langle [\nu]\alpha L \parallel a^\dagger_l \parallel [\nu_1]\alpha_1 L_1\rangle \,, \tag{7-306}$$

while the two–body CFP in (7-168a) is related to the reduced matrix element of pair creation operator in the generalized quantization

$$\langle l^{n-2}[\nu_1]\alpha_1 L_1, l^2 L_2|\}l^n[\nu]\alpha L\rangle^{\nu'} = (-1)^{2l-L}\langle [\nu]\alpha L \parallel [a^\dagger_l a^\dagger_l]^{L_2} \parallel [\nu_1]\alpha_1 L_1\rangle^{\nu'} \,, \tag{7-307}$$

where the factor $(-1)^{2l-L}$ comes from the fact that acting on the state of $n-2$ particles the operator $[a^\dagger_l a^\dagger_l]^{L_2}$ create a two–particle state

$$[\psi_l(n)\psi_l(n-1)]^{L_2} = (-1)^{2l-L_2}\,[\psi_l(n-1)\psi_l(n)]^{L_2} \,.$$

To verify (7-307), we use the following formula

$$\begin{aligned}\langle [\nu]\alpha L \parallel [Y_{k_1} \times Z_{k_2}]^k \parallel [\nu_1]\alpha_1 L_1\rangle^{\nu'} &= \sum_{\alpha' L'} (-1)^{k_1+k_2-k} U(L_1 k_2 L k_1; L' k) \\ &\times \langle [\nu]\alpha L \parallel Y_{k_1} \parallel [\nu']\alpha' L'\rangle\langle [\nu']\alpha' L' \parallel Z_{k_2} \parallel [\nu_1]\alpha_1 L_1\rangle \,,\end{aligned} \tag{7-308}$$

to calculate the matrix elements of $[a^\dagger_l a^\dagger_l]^{L_2}$,

$$\begin{aligned}(-1)^{2l-L_2}\langle [\nu]\alpha L \parallel [a^\dagger_l a^\dagger_l]^{L_2} \parallel [\nu_1]\alpha_1 L_1\rangle^{\nu'} &= \sum_{\alpha' L'} U(L_1 l L l; L' L_2) \\ &\times \langle [\nu]\alpha L \parallel a^\dagger_l \parallel [\nu']\alpha' L'\rangle\langle [\nu']\alpha' L' \parallel a^\dagger_l \parallel [\nu_1]\alpha_1 L_1\rangle,\end{aligned} \tag{7-309}$$

which is just (7-168b).

From (7-306) and (7-307) it is seen that the CFP in partial spaces can be expressed as the reduced matrix elements of the hybrid operators.

7.20.3 The relation between the generalized and second quantizations

Notice that in (7-303) the the irrep label for the intermediate states is a summation index. For example, if $[\nu'] = [1^{n-1}]$, then ν has two possible values, $[1^n]$ and $[21^{n-2}]$. In the following we will use the phrase "in the totally anti–symmetric (symmetric) space". It means that all the initial, final and intermediate states are totally anti–symmetric (symmetric). To implement such a restriction it is convenient to introduce the operator $\hat{a}^\dagger_\alpha$ which is equal to the product of the anti–symmetrizer $P^{[1^n]}$ (or symmetrizer $P^{[n]}$ (4-68b)) with $a^\dagger_\alpha$,

$$\hat{a}^\dagger_\alpha = P^{[1^n]}a^\dagger_\alpha, \;\; \hat{a}^\dagger_\alpha|[1^{n-1}]w) = \sum_w |[1^n]w)([1^n]w|a^\dagger_\alpha|[1^{n-1}]w') \tag{7-310}$$

We now turn to the total symmetric (or anti–symmetric) space, and the single–particle state $\alpha, \beta, \ldots$, could be something like $lm_l sm_s tm_t$, or $jm_j tm_t$, for example. It is well known that the matrix element of a one–body operator between two totally symmetric (or anti–symmetric)

n–particle states is equal to n times that of the one–body operator referring to a specific, say, the nth particle. That is, we have

$$([n]w|C_\alpha^\dagger C_\beta|[n]w') = n([n]w|a_\alpha^\dagger a_\beta|[n]w'). \tag{7-311}$$

From (7-310) and (7-311) we obtain the relation between the second and generalized quantizations,

$$C_\alpha^\dagger|[n-1]w') = \sqrt{n}\hat{a}_\alpha^\dagger|[n-1]w'),\ C_\alpha|[n]w') = \sqrt{n}a_\alpha|[n]w). \tag{7-312}$$

From (7-312) we immediately obtain the relations between the matrix elements of the operators in these two formalisms:

$$\begin{aligned}
([n]w|C_\alpha^\dagger|[n-1]w') &= \sqrt{n}([n]w|a_\alpha^\dagger|[n-1]w'),\\
([n]w|C_\alpha^\dagger C_\beta^\dagger|[n-2]w'') &= \sqrt{n(n-1)}([n]w|a_\alpha^\dagger a_\beta^\dagger|[n-2]w'')\\
([n]w|C_\alpha^\dagger C_\beta^\dagger C_\gamma C_\delta|[n]\bar{w}) &= n(n-1)([n]w|a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta|[n]\bar{w}),\\
([n]w|C_\alpha^\dagger C_\beta^\dagger C_\gamma|[n-1]w') &= (n-1)\sqrt{n}([n]w|a_\alpha^\dagger a_\beta^\dagger a_\gamma|[n-1]w'),\\
([n]w|C_\alpha^\dagger C_\gamma C_\delta|[n+1]w^0) &= n\sqrt{n+1}([n]w|a_\alpha^\dagger a_\gamma a_\delta|[n+1]w^0).
\end{aligned} \tag{7-313}$$

From (7-313) we know that in the totally symmetric (anti–symmetric) space, $a_\alpha^\dagger$ and $a_\beta^\dagger$ commute (anticommute),

$$\begin{aligned}
&[a_\alpha^\dagger, a_\beta^\dagger] = 0, \quad \text{in totally symmetric space}\\
&\{a_\alpha^\dagger, a_\beta^\dagger\} = 0, \quad \text{in totally anti–symmetric space}
\end{aligned} \tag{7-314}$$

From (7-313) and (7-314) we conclude that in the totally symmetric (anti–symmetric) spaces, the hybrid operators (apart from nonessential factors) reduce to the boson (fermion) operators, and in this sense the generalized quantization is an extension of the second quantization.

In summary, we compare the three quantizations:

The first quantization: It is applicable to both partial space and total spaces. Both states and operators have particle indices, and the operators obey the commutators,

$$[a_\alpha^\dagger(i), a_\alpha^\dagger(j)] = 0,\ [a_\alpha(i), a_\alpha^\dagger(j)] = \delta_{\alpha\beta}\delta_{ij}.$$

The second quantization: It is applicable only to total space. Both states and operators do not have particle indices, and the operators obey either the bosonic or fermionic commutators.

The generalized quantization: It is applicable to both partial and total spaces. The states have particle indices while the operators have implicit particle indices (creates or annihilates the last particle). In the totally symmetric (anti–symmetric) spaces, the generalized quantization reduces to second quantization.

We discuss the application of the generalized quantization to the nuclear shell model in Sec. 9.1.2.

Chapter 8

The Point Groups

This chapter deals with the elementary concepts and definitions relating to point groups, with emphasis on the algebraic solutions for the dihedral groups D_n and cubic groups by the EFM for both the single–valued and double–valued representations. It will be shown that with the algebraic expression of the projection operator, the projection operator method becomes extremely simple and powerful. We introduce the so–called representation group, which is very useful for treating the double–valued (d–v) reps of the point groups and space groups. Readers are referred to McWeeny (1963), Bradley & Cracknell (1972) and Chen & Fan (1998) for more detailed presentations on the point groups. We shall use Schönflies notation.

8.1. Basic Operations of Point Groups and Their Faithful Representations

Many microscopic and macroscopic objects (or systems) exhibit some form of symmetry. For example, nuclei, atoms, molecules, snowflakes, equilateral triangles, hexagonal nuts, cubes, regular pyramids and prisms. The operation which brings a system into a position indistinguishable from that which it originally occupied is called a *symmetry operation* of the system. The operation does not change the distance between any two points inside the system. All such operations form a group, called the *symmetry group* of the system.

The symmetry group of a finite system is called a *point group*, since all the symmetry operations must leave at least one point of the system unmoved.

The Cartesian coordinates x, y, z carry the fundamental rep of the three–dimensional orthogonal group O_3. Since any point group is a subgroup of O_3, the coordinates x, y, z also carry a rep D for the point group, which is a *faithful* but in general reducible rep of the point group G.

The atoms in a molecule are said to be *equivalent* if they exchange positions with one another under a symmetry operation. Equivalent atoms are necessarily chemically identical.

We first use the faithful representation of point groups to deduce some useful relations of the basic operators, which are valid only for single-valued (s–v) reps, and then in Sec. 8.11.3 extend these relations so that they are valid for both s–v and d–v reps. Some relations in this subsection are attached with the tag "for s–v", which means that they are valid only for s–v reps, while those without tags are valid for both s–v and d–v reps.

The basic operations of point groups are as follows:

1. *Proper* (or *pure*) rotations

A rotation through angle $2\pi/l$ about an axis $\mathbf{n}$ is designated as $C_l^{\mathbf{n}}$. The maximum l is called the *order* (or *fold*) of the rotation axis. A point group may contain several rotation axes. The one with the highest order is called the principal axis. One usually chooses the principal axis as

the z–axis. From (2-60b) we get the faithful rep of $C_n^z \equiv C_{nz}$,

$$D(C_{nz}) = \begin{pmatrix} \cos\frac{2\pi}{n} & -\sin\frac{2\pi}{n} & 0 \\ \sin\frac{2\pi}{n} & \cos\frac{2\pi}{n} & 0 \\ 0 & 0 & 1 \end{pmatrix} . \tag{8-1}$$

We often use the notations

$$C_{nz}^{+} \equiv C_{nz}, \quad C_{nz}^{-} \equiv C_{nz}^{-1} .$$

To simplify notation, the subscript z in C_{nz} will be ignored when no confusion will arise. We have

$$C_n = \exp\left(-\tfrac{2\pi i}{n} J_z\right) = C_{nm}^{m} , \quad C_n^m \equiv (C_n)^m = C_{n/m} = \exp\left(-\tfrac{2m\pi i}{n} J_z\right) , \tag{8-2a}$$

$$C_n^{n-1} = C_n^{-1} , \quad C_n^n = R_z(2\pi) = e , \quad \text{for s-v only.} \tag{8-2b}$$

The set $\{C_{nz}^k : k = 1, 2, \ldots, n\}$ forms the cyclic group $\mathcal{C}_n$. Evidently, the determinant of the natural rep of any proper rotation is equal to $+1$.

We use $C_2^{(\varphi)} \equiv C_2^{\mathbf{n}_\varphi}$ to denote a two–fold rotation about the axis $\mathbf{n}_\varphi$ in the xy–plane with azimuth angle φ, (see Fig. 8.1). Therefore

$$C_2^{(0^\circ)} = C_{2x}, \; C_2^{(90^\circ)} = C_{2y}.$$

Clearly we have

$$D(C_{2x}) = \{1, -1, -1\}_{\text{diag}}, \quad D(C_{2y}) = \{-1, 1, -1\}_{\text{diag}}, \quad D(C_{2z}) = \{-1, -1, 1\}_{\text{diag}}, \tag{8-3a}$$

where $\{a, b, c\}_{\text{diag}}$ represents a diagonal matrix, and

$$C_2^{(\varphi)} \equiv C_2^{\mathbf{n}_\varphi} = R_z(\varphi) C_{2x} R_z^{-1}(\varphi) , \tag{8-4}$$

where $R_z(\varphi)$ is a rotation through an angle φ about the z–axis. We also have

$$C_{2x}^2 = C_{2y}^2 = C_{2z}^2 = 1, \quad C_2^{\mathbf{n}} = C_2^{-\mathbf{n}}, \quad \text{for s-v only.} \tag{8-3b}$$

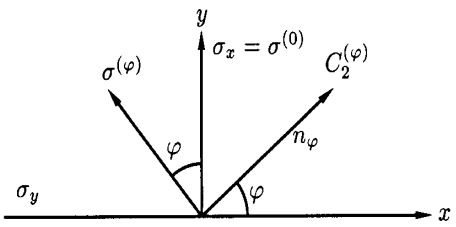


Fig. 8.1. Rotation and reflection operators.

Two operations A and B of a group G are said to be *equivalent* if there exists an operation C in G such that

$$B = CAC^{-1} . \tag{8-5a}$$

If there is a rotation or a reflection C in the group G which carries the rotation axis $\mathbf{n}$ into $\mathbf{n}'$,

$$R_{\mathbf{n}'}(\omega) = C R_{\mathbf{n}}(\omega) C^{-1} , \tag{8-5b}$$

then the axes $\mathbf{n}$ and $\mathbf{n}'$ are said to be *equivalent*. If $\mathbf{n}$ and $-\mathbf{n}$ are *equivalent* , then the axis $\mathbf{n}$ is said to be *bilateral* or *two sided* . Obviously, if there is a two–fold axis (or a reflection plane) perpendicular to the axis $\mathbf{n}$, then $\mathbf{n}$ is bilateral.

For example, in Fig. 8.1, if $R_z(\varphi)$ is an element of the point group G, then $C_2^{\mathbf{n}_\varphi}$ and C_{2x} are equivalent operations, while $\mathbf{n}_\varphi$ and x are equivalent axes. From (5-32), we obtain the faithful rep of $R_z(\varphi)$,

$$D(R_z(\varphi)) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} . \tag{8-6}$$

From (8-3), (8-4) and (8-6) we immediately have

$$D(C_2^{(\varphi)}) = \begin{pmatrix} \cos 2\varphi & \sin 2\varphi & 0 \\ \sin 2\varphi & -\cos 2\varphi & 0 \\ 0 & 0 & -1 \end{pmatrix} , \tag{8-7}$$

and from (8-3) and (8-7) we see that $D(C_2^{(\varphi)})D(C_{2x}) = D(R_z(2\varphi))$. Since D is a faithful rep of G, we have the important relation:

$$C_2^{(\varphi)} C_{2x} = R_z(2\varphi) , \quad \text{for s–v only,} \tag{8-8}$$

namely, successive rotations through angle π about two axes making an angle φ with one another is equivalent to a rotation through angle 2φ about an axis perpendicular to the first two axes. Therefore if a group G has two–fold axes making an angle φ with one another, then there must exist an n–fold axis with $n = 2\pi/2\varphi = \pi/\varphi$. Conversely, if a group G has an n–fold axis and one two–fold axis, then there must exist n two–fold axes, with angle $\varphi = \pi/n$ between any two adjacent axes.

From (8-3) it is seen that $[D(C_{2x}), D(C_{2y})] = 0$. Thus

$$[C_{2x}, C_{2y}] = 0 , \quad \text{for s–v only,} \tag{8-9}$$

namely, two rotations through angle π about perpendicular axes commute with one another. According to the fact that under the rotation C_{2x} the operator J_z goes over to $-J_z$, from (8-2) we have

$$C_{2x} C_{nz} C_{2x}^{-1} = C_{nz}^{-1} . \tag{8-10}$$

2. *The inversion I*

This inversion transforms x, y, z into $-x, -y, -z$, and in the faithful rep we have

$$D(I) = \{-1, -1, -1\}_{\text{diag}} . \tag{8-11}$$

Since $D(I)$ equals a negative unit matrix, the inversion I commutes with any elements of the point group.

3. *Reflections*

A reflection is a product of a two–fold rotation and the inversion,

$$\sigma_i = C_{2i} I = I C_{2i}, \quad i = x, y, z, \tag{8-12a}$$

where σ_x is a reflection plane with its normal in the x direction. Therefore in any representation $\mathcal{D}$ we have

$$\mathcal{D}(\sigma_i) = \mathcal{D}(I)\mathcal{D}(C_{2i}) = \pm\mathcal{D}(C_{2i}) . \tag{8-12b}$$

From (8-3) and (8-11) we have

$$D(\sigma_x) = \{-1, 1, 1\}_{\text{diag}}, \quad D(\sigma_y) = \{1, -1, 1\}_{\text{diag}}, \quad D(\sigma_z) = \{1, 1, -1\}_{\text{diag}}, \tag{8-13a}$$

$$\det(D(\sigma_i)) = -1\ , \quad i = x, y, z\ . \tag{8-13b}$$

Below we often use $\sigma^{\mathbf{n}}$ to denote a reflection plane with $\mathbf{n}$ as its normal direction. Similar to (8-3b) we have

$$\sigma_i^2 = 1, \quad \sigma^{\mathbf{n}} = \sigma^{-\mathbf{n}}, \quad \sigma_x = \sigma_{-x} \cdots, \text{ for s-v only.} \tag{8-13c}$$

From (8-3b) and (8-12a),

$$I = \sigma_i C_{2i} = C_{2i}\sigma_i\ , \text{ for s-v only.} \tag{8-13d}$$

3a. *Reflection across a horizontal plane*

The reflection σ_z is called a reflection across a horizontal plane, denoted σ_h. According to (8-6) and (8-13a) we have

$$[\sigma_z, R_z(\varphi)] = 0\ . \tag{8-14a}$$

That is, a rotation commutes with the reflection across a plane which is perpendicular to the rotation axis. From (8-14a) we have

$$\sigma_z C_{nz} \sigma_z^{-1} = C_{nz}\ . \tag{8-14b}$$

Any planar molecule has σ_h symmetry with the molecular plane as the reflection plane.

3b. *Reflection across a vertical plane* σ_v

The operation σ_v denotes a reflection across a plane containing the principal axis. Suppose that a group G has two vertical reflection planes, $\sigma^{\mathbf{n}_\varphi} = \sigma^{(\varphi)}$ and $\sigma_x = \sigma^{(0^\circ)}$, φ being the angle between the normal $\mathbf{n}_\varphi$ and the x axis (or between the intersection of $\sigma^{\mathbf{n}_\varphi}$ with the xy–plane and the y axis (see Fig. 8.1). Multiplying both sides of (8-4) with I gives

$$\sigma^{(\varphi)} = \sigma^{\mathbf{n}_\varphi} = C_2^{(\varphi)} I = R_z(\varphi)\sigma_x R_z(-\varphi)\ . \tag{8-15}$$

Notice that the reflection $\sigma^{(\varphi)}$ defined in the first edition of this book, denoted $\sigma^{(\varphi)}|_{\text{wspc-89}}$, is related to the new definition of Fig. 8.1 by

$$\sigma^{(\varphi)}|_{\text{wspc-89}} = \sigma^{(\varphi+\pi/2)}\ ,$$

Combining (8-7), (8-11) and (8-15) we get

$$D(\sigma^{(\varphi)}) = -D(C_2^{(\varphi)}) = -\begin{pmatrix} \cos 2\varphi & \sin 2\varphi & 0 \\ \sin 2\varphi & -\cos 2\varphi & 0 \\ 0 & 0 & -1 \end{pmatrix}\ . \tag{8-16}$$

Multiplying (8-8) with $I^2 = 1$ we get

$$\sigma^{(\varphi)}\sigma^{(0)} = R_z(2\varphi)\ , \quad \text{for s-v only.} \tag{8-17}$$

That is, the product of two vertical reflections across planes making an angle φ with each other is equivalent to a rotation through an angle 2φ about the z–axis.

Consequently, if a group G has two vertical reflection planes making an angle φ with each other, then there must exist an n–fold axis with $n = \pi/\varphi$. Conversely, if a group G has an n–fold axis and a vertical reflection plane, then there must exist n vertical reflection planes with angle $\varphi = \pi/n$ between any two adjacent planes.

From (8-13a) we can infer that

$$[\sigma_x, \sigma_y] = 0\ , \quad \text{for s-v only.} \tag{8-18}$$

This shows that two reflection operations commute if their reflection planes are perpendicular.

If $R_z(\varphi)$ in (8-15) is an element of the group G, then $\sigma^{\mathbf{n}_\varphi}$ and σ_x are said to be *equivalent planes.*

4. *Improper rotations*

The improper rotations, or rotation–reflections, S_{nz} are defined as products of a proper rotation and a horizontal reflection,

$$S_{nz} = C_{nz}\sigma_h = \sigma_h C_{nz} = C_{nz}\sigma_z \ , \quad \text{for s–v only.} \tag{8-19}$$

From (8-1) and (8-13a) we find the faithful rep of the improper rotation,

$$D(S_{nz}) = \begin{pmatrix} \cos\frac{2\pi}{n} & -\sin\frac{2\pi}{n} & 0 \\ \sin\frac{2\pi}{n} & \cos\frac{2\pi}{n} & 0 \\ 0 & 0 & -1 \end{pmatrix} . \tag{8-20}$$

Using (8-2) we get

$$C_{nz}C_{2z} = C_{2n,z}^{n+2} . \tag{8-21}$$

For s–v reps

$$C_{2n,z}^{n+2} = (C_{2n,z}^{n-2})^{-1} . \tag{8-22}$$

It follows that

$$S_3^+ = C_6^- I, \quad S_4^+ = C_4^- I, \quad S_6^+ = C_3^- I . \tag{8-23}$$

From (8-19) we have

$$S_{nz}^k = (S_{nz})^k = \begin{cases} C_{nz}^k \\ C_{nz}^k\sigma_h \end{cases} , \quad \text{for } k = \begin{cases} \text{even} \\ \text{odd} \end{cases} . \tag{8-24a}$$

$$S_{nz}^n = \begin{cases} e \\ \sigma_h \end{cases} , \quad \text{for } n = \begin{cases} \text{odd} \\ \text{even} \end{cases} . \tag{8-24b}$$

Therefore when n is even, $\{S_{nz}^k : k = 1, 2, \ldots, n\}$ forms a group, denoted by S_n, and when n = odd, $\{S_{nz}^k : k = 1, 2, \ldots, 2n\}$ forms a group, denoted by C_{nh}, both being Abelian.

$$S_{2n} = \{S_{2n,z}^k : k = 0, 1, \ldots, 2n-1\}, \quad n = 1, 2, 3, \cdots , \tag{8-25a}$$

$$C_{nh} = \{S_{nz}^k : k = 0, 1, \ldots, 2n-1\}, \quad n = \text{odd}. \tag{8-25b}$$

From (8-19) and (8-13d) we get

$$S_{nz}^{n/2} = C_{nz}^{n/2}\sigma_h = C_{2z}\sigma_z = I, \quad \text{for } \tfrac{n}{2} = \text{odd} . \tag{8-25c}$$

Therefore, the groups S_{2n} with odd n = must contain the inversion, namely

$$S_{2n} = C_n \times C_i, \quad \text{for } n = \text{ odd}.$$

A rotation axis or a reflection plane is called a *symmetry element* of the point group.

Equation (8-5) tells us that a set of equivalent operations constitutes a class of a point group. Concerning the classes of point groups we have the following obvious results.

1. The identity operation and inversion I, each forms a class by itself. For the dihedral groups the horizontal reflection σ_h forms a class by itself.

2. Proper (or improper) rotations through the same angle about equivalent axes belong to the same class.

3. Equivalent reflections belong to the same class.

4. For a two–sided axis, a rotation (proper or improper) and its inverse belong to the same class.

For a point group, we often use the symbol "nX" to designate a class, or a class operator, where n is the number of elements in the class and X is an operator belonging to the class.

8.2. Some Commonly Used Point Groups

The classification and generators of some of the most commonly used point groups are listed in Table 8.2-1. McWeeny (1963) listed the group elements and classes for them.

Table 8.2-1. Some commonly used point groups. We use e. and o. to represent even and odd respectively.

group	order	class numbers	inter-relations	generators	symmetry objects
$\mathcal{C}_1$	1	1		e	
$\mathcal{C}_i$	2	2		I	
$\mathcal{C}_s$	2	2	$\mathcal{C}_s = \mathcal{C}_{1h}$	σ_h	
C_n	n	n		C_{nz}	
C_{nv}	$2n$	$\begin{cases} 3+n/2 & \text{e.n} \\ (3+n)/2 & \text{o.n} \end{cases}$	$C_{nv} \sim D_n$	C_{nz}, σ_x	regular n-sided pyramid
C_{nh}	$2n$	$2n$	$C_{nh} = \begin{cases} C_n \times \mathcal{C}_s, \\ C_n \times \mathcal{C}_i, & \text{e.n} \end{cases}$	C_{nz}, σ_h	
S_{2n}	$2n$	$2n$	$S_{2n} = C_n \times \mathcal{C}_i$, o.n	$S_{2n,z}$	
D_n	$2n$	$\begin{cases} (n+6)/2 & \text{e.n} \\ (n+3)/2 & \text{o.n} \end{cases}$	$D_n \sim C_{nv}$	C_{nz}, C_x	
D_{nh}	$4n$	$\begin{cases} n+6 & \text{e.n} \\ n+3 & \text{o.n} \end{cases}$	$D_{nh} = \begin{cases} D_n \times \mathcal{C}_s, \\ D_n \times \mathcal{C}_i, & \text{e.n} \end{cases}$	C_{nz}, C_{2x}, σ_h	regular n-sided prism
D_{nd}	$4n$	$n+3$	$D_{nd} = \begin{cases} C_{nv} \times \mathcal{C}_i \\ D_n \times \mathcal{C}_i, \end{cases}$ o.n	C_{nz}, C_{2x}, σ_x	
T	12	4		C_{2z}, C_{31}	cube (proper rotations only)
T_d	24	5		S_{4z}, C_{31}	tetrahedron
T_h	24	8	$T_h = T \times \mathcal{C}_i$	C_{2z}, C_{31}, I	
O	24	5		C_{4z}, C_{31}	cube, (octahedron, proper rot. only)
O_h	48	10	$O_h = O \times \mathcal{C}_i$	C_{4z}, C_{31}, I	cube, octahedron

Now let us discuss the construction of point groups. In the following we often use the generator of a cyclic group in italic symbol to denote the cyclic group, for example,

$$\mathcal{C}_{2x} = \{e, C_{2x}\}, \quad \mathcal{C}_{2b} = \{e, C_{2b}\}, \quad \mathcal{C}_{sz} = \{e, \sigma_z\}, \quad \mathcal{C}_{sa} = \{e, \sigma_{da}\}.$$

The simplest point groups are the inversion group $\mathcal{C}_i = (e, I)$ and reflection group $\mathcal{C}_s \equiv \mathcal{C}_{sz} = (e, \sigma_h)$. The next simplest groups are the cyclic groups $C_n = \{C_{nz}^k : k = 0, 1, \cdots, n-1\}$, S_{2n} and C_{nh}. The group C_{nh} is a direct product of C_n and $\mathcal{C}_s$

$$C_{nh} = C_n \times \mathcal{C}_s. \tag{8-26}$$

When n = even, $C_{nh} = C_n \times \mathcal{C}_i$, and when n = odd, C_{nh} can be expressed as in (8-25b).

The simplest non-Abelian point groups are *axial groups* or *dihedral groups* D_n, C_{nv}, D_{nd} and D_{nh}. The group D_n is obtained by adding a two-fold axis C_{2x} to C_n, and the group C_{nv} is obtained by adding a reflection σ_x to C_n. They are semi-direct products of C_n with $\mathcal{C}_{2x}$ and $\mathcal{C}_{sx}$, respectively,

$$D_n = C_n \wedge \mathcal{C}_{2x}, \quad C_{nv} = C_n \wedge \mathcal{C}_{sx}. \tag{8-27a}$$

The group D_{nd} is obtained by adding to D_n a vertical reflection plane which bisect the angle between two adjacent horizontal two-fold axes, which implies that there are n vertical planes and each of them bisects the angle between two adjacent two-fold axes.

The group D_{nh} is obtained by adding to D_n n vertical reflection planes whose intersections with the x–y plane coincide with the n horizontal two-fold axes.

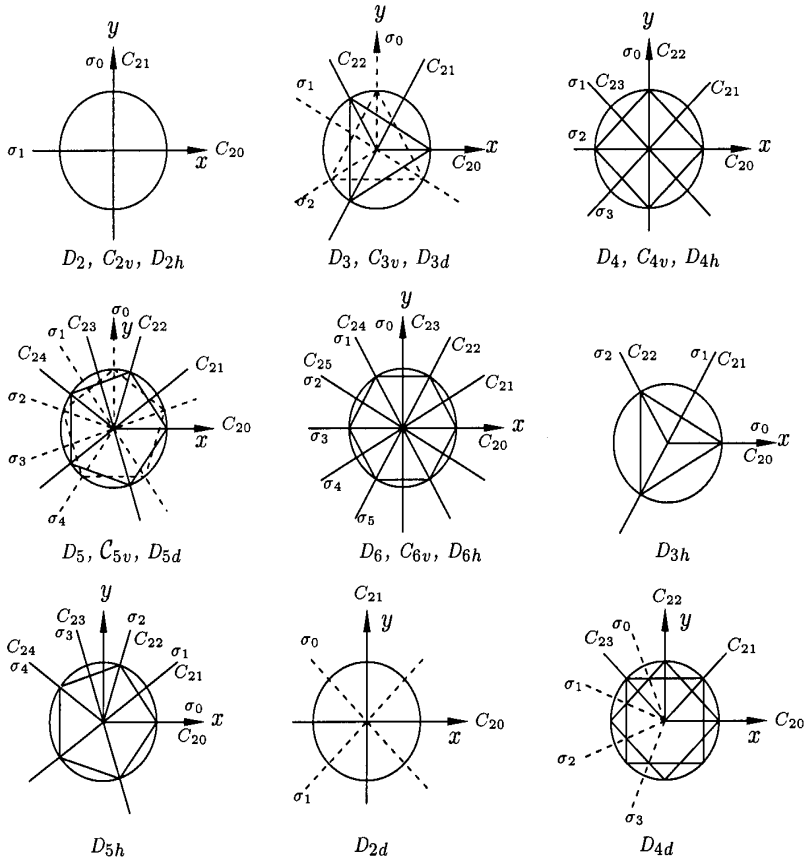


Fig. 8.2-1. Two-fold axes and reflection planes of selected dihedral groups.

The two-fold axes and reflection planes of these dihedral groups are shown in Fig. 8.2-1. The diagrams for $D_n = \{C_{2i}, \cdots\}, C_{nv} = \{\sigma_i, \cdots\}$, and $D_{nh} = \{C_{2i}, \sigma_i, \cdots\}$ for n = even or $D_{nd} = \{C_{2i}, \sigma_i, \cdots\}$ for n = odd are shown in the same figure. It is seen that for D_{nh} with even n or for D_{nd} with odd n, the n vertical reflection planes are perpendicular to the n two-fold axes. For these cases we have $\sigma_k = C_{2k}I, k = 1, 2, \cdots, n$. Therefore there is the inversion in the group; $D_{nh} = D_n \times C_i$ for even n and $D_{nd} = D_n \times C_i$ for odd n. In the following we only need to consider the dihedral groups D_n, C_{nv}, D_{nh} (odd n) and D_{nd} (even n). The group D_{nh} (odd n) is a semi-direct product of D_n and $\{e, \sigma_y\}$,

$$D_{nh} = D_n \wedge C_{sy}, \tag{8-27b}$$

while the group D_{nd} (even n) is a semi-direct product of D_n and $\{e, \sigma_0\}$,

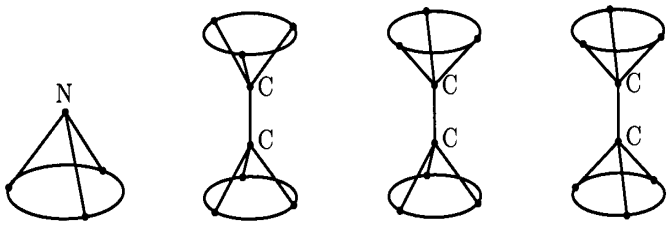
$$D_{nd} = D_n \wedge \{e, \sigma_0\}, \ \sigma_0 = C_{2n,z}\sigma_x. \tag{8-27c}$$

Notice that the relation $D_{nh} = D_n \times C_s$ shown in Table 8.2-1 holds only for s-v case, and for d-v case D_{nh} is merely a semi-direct product of D_n and C_s, $D_{nh} = D_n \wedge C_s$.

Figure 8.2-2 gives the four types of molecules with the symmetries C_{3v}, D_3, D_{3h} and D_{3d}.

Tetrahedral groups:

The group T is the pure rotation group of a regular tetrahedron as shown in Figure 8.2-3 where a tetrahedron is inscribed in a cube. The group T is obtained by adding a three-fold axis



NH_3 C_{3v} | C_2H_6 D_3 | C_2H_6 D_{3h} | C_2H_6 D_{3d}

Fig. 8.2-2. Molecules having the C_{3v}, D_3, D_{3h} and D_{3d} symmetries. The unlabelled points represent hydrogen atoms.

to D_2,

$$T = D_2 \wedge C_3, \quad C_3 = \{e, C_{31}^+, C_{31}^-\}. \tag{8-27d}$$

It is seen that T has three 2-fold axes passing the midpoints of two non-adjacent sides, C_{2x}, C_{2y} and C_{2z} and four 3-fold axes $C_{3i}, i = 1, 2, 3, 4$ (starting from the origin and pointing to the four corners 1,2,3,4 of the tetrahedron).

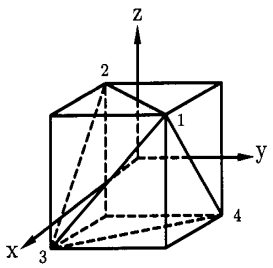


Fig. 8.2-3. The tetrahedron.

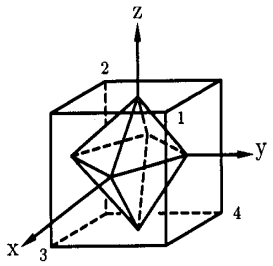


Fig. 8.2-4. The octahedron.

Using the transformations of the vertices under the symmetry operations, it is easy to find the correspondence between the point group and permutation group, shown in Table 8.2-2.

From the first half of Table 8.2-2, one sees that T is isomorphic to the alternating group $\mathcal{A}_4$ and has four classes,

$$C_1 = e,\ C_2 = C_{2x} + C_{2y} + C_{2z},\ C_3 = C_{31}^+ + C_{32}^+ + C_{33}^+ + C_{34}^+,\ C_4 = C_3^\dagger\ .$$

We can obtain products of the symmetry operations by means of the multiplication rule of the permutation group. For example, from (234)(143)=(123), we know that $C_{31}^+ C_{32}^+ = C_{34}^{-1}$.

Table 8.2-2 also shows that e, C_{2x}, C_{2y}, and C_{2z} form a subgroup D_2 of T, and that D_2 is isomorphic to the four-group.

The group T_d is the symmetry group of a regular tetrahedron. In addition to the twelve elements of the group T, T_d contains another twelve elements which can be expressed as $S_{4z}T$. From Table 8.2-2 one sees that T_d is isomorphic to the permutation group S_4 and has five classes,

$$C_1 = e, C_2 = C_{2x} + C_{2y} + C_{2z}, C_3 = C_{31}^+ + \cdots + C_{34}^-, C_4 = S_{4x}^+ + \cdots + S_{4z}^-, C_5 = \sigma_{da} + \cdots + \sigma_{df}.$$

The reflection plane σ_{da} corresponding to the permutation (12) contains the side (34) and the midpoint of the side (12). Under this reflection, the vertices 1 and 2 are interchanged.

Table 8.2-2. The isomorphism $T \sim \mathcal{A}_4$, and $T_d \sim O \sim S_4$.

e	C_{2x}	C_{2y}	C_{2z}	C_{31}^{+}	C_{32}^{+}	C_{33}^{+}	C_{34}^{+}	C_{31}^{-}	C_{32}^{-}	C_{33}^{-}	C_{34}^{-}
e	(13)(24)	(12)(34)	(13)(24)	(234)	(143)	(124)	(132)	(243)	(134)	(142)	(123)

S_{4x}^{+} C_{4x}^{-}	S_{4y}^{+} C_{4y}^{-}	S_{4z}^{+} C_{4z}^{-}	S_{4x}^{-} C_{4x}^{+}	S_{4y}^{-} C_{4y}^{+}	S_{4z}^{-} C_{4z}^{+}	σ_{da} C_{2a}	σ_{db} C_{2b}	σ_{dc} C_{2c}	σ_{dd} C_{2d}	σ_{de} C_{2e}	σ_{df} C_{2f}
(1234)	(1342)	(1423)	(1432)	(1243)	(1324)	(12)	(34)	(14)	(13)	(23)	(24)

Octahedral groups:

The group O is the pure rotation group of a regular octahedron, or a cube. The former can be inscribed in the latter (see Fig. 8.2-4). The group O is a semi–direct product group of T and C_{2a},

$$O = T \wedge C_{2a}. \tag{8-27e}$$

The rotation axes of the group O are shown in Fig. 8.2-5, which are used in Bradley & Cracknell (1972). Another commonly used notation is due to McWeeny (1963). The correspondence between the two are shown in Table 8.2-3.

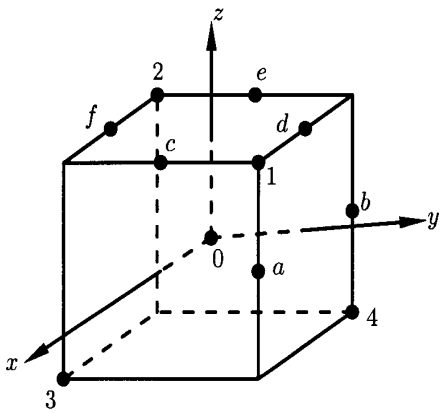


Fig. 8.2-5 The symmetry elements of O. The four three–fold axes C_{31}^{+}, C_{32}^{+}, C_{33}^{+}, C_{34}^{+} are $\underline{01}, \underline{02}, \underline{03}, \underline{04}$, and the six two–fold axes C_{2a}, C_{2b}, C_{2c}, C_{2d}, C_{2e}, C_{2f} are $\underline{0a}, \underline{0b}, \underline{0c}, \underline{0d}, \underline{0e}, \underline{0f}$, respectively.

Table 8.2-3. Correspondence between Bradley and McWeeny notation.

C_{2a} C_2^{xy}	C_{2b} $C_2^{x\bar{y}}$	C_{2c} C_2^{xz}	C_{2d} C_2^{yz}	C_{2e} $C_2^{x\bar{z}}$	C_{2f} $C_2^{y\bar{z}}$	C_{31}^{+} C_3^{xyz}	C_{32}^{+} $C_3^{\bar{x}yz}$	C_{33}^{+} $C_3^{x\bar{y}z}$	C_{34}^{+} $C_3^{\bar{x}y\bar{z}}$

In McWeeny notation, C_2^{xy} is a two–fold axis lying in the x–y plane and having the same angle with respect to the axes x and y, while $C_3^{\bar{x}yz}$ is a three–fold axis passing the origin and having equal angles with respect to the $\bar{x}(=-x), y$ and $\bar{z}(=-z)$ axes.

The group O contains the tetrahedral group T and is isomorphic to T_d and S_4, as shown in Table 8.2-2. The group O has the following symmetry operations:

1. Three 4–fold axes, C_{4x}, C_{4y} and C_{4z}.

2. Four 3–fold axes $C_{3i}, i = 1, 2, 3, 4$, passing the center of two opposite faces of the octahedron, or equivalently, joining the nearest and furtherest cube corners, which are the same as in the group T.

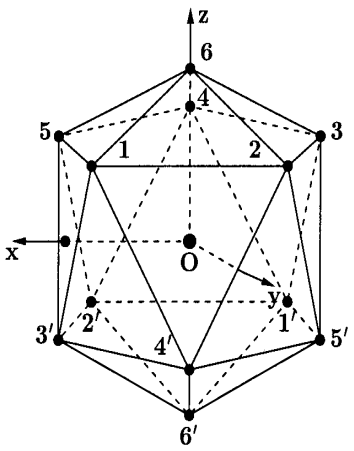


Fig. 8.2-6 The icosahedron.

3. Six 2–fold axes passing through the midpoints of two opposite sides of the octahedron, such as $C_{2a}, \ldots, C_{2f}$ (see Table 8.2-3).

The 24 elements of the group O fall into five classes:

$$C_1 = e, C_2 = C_{2x} + C_{2y} + C_{2z}, C_3 = C_{31}^{+} + \cdots + C_{34}^{-}, C_4 = C_{4x}^{+} + \cdots + C_{4z}^{-}, C_5 = C_{2a} + \cdots C_{2f}.$$

From (8-12) we have

$$\sigma_{di} = C_{2i} I, \quad i = a, b, c, d, e, f. \tag{8-28}$$

The group O_h is the symmetry group of a regular octahedron. By annexing the inversion I to the group O we get the group O_h with 48 elements: $O_h = (e \oplus I)O$.

Icosahedral groups:

The group I is the pure rotation group of an icosahedron, or of a dodecahedron inscribed in an icosahedron. The vertices of an icosahedron are labelled as in Fig. 8-2-6. The vertices of the upper (lower) part are labelled 1–6 (1′–6′). The group I has

1. 6 five–fold axes (joining the two opposite vertices), $C_{5,j}$, $j = 1, \cdots, 6$,
2. 10 three–fold axes (joining the center of two opposite faces), $C_{3,j}$, $j = 1, \cdots, 10$,
3. 15 two–fold axes (joining the midpoints of the opposite edges), $C_{2,j}$, $j = 1, \cdots, 15$,

The group I_h is the symmetry group of an icosahedron. $I_h = I \times C_i$.

Crystal, or crystallographic, point groups: In crystals, there are only 32 possible crystal point groups (see Sec. 10.4), namely $C_n, C_{nh}, C_{nv}, D_n, D_{nh}$, for $n = 2, 3, 4, 6$; D_{2d}, D_{3d}, C_1, C_i, C_s, S_4, S_6, T, T_h, T_d, O and O_h.

The group tables for the point group O can be found from Table 10.24-1.

Molecular point groups: In addition to the 32 crystal point groups, there are also the following point groups for molecules: $C_5, C_7, C_8, C_{5h}, C_{5v}, D_5, D_{5h}, D_{5d}, D_{4d}, D_{6d}, D_{8h}, D_{\infty h}, C_{\infty v}$, and the icosahedral groups I and I_h. The group $C_{\infty v}$ is the symmetry group of linear molecules without symmetry centers, such as CO (see Fig. 8.2-7), and $D_{\infty h}$ is the symmetry group of linear molecules with symmetry centers, such as H_2, O_2, or CO_2 (see Fig. 8.2-8). The groups $C_{\infty v}$ and $D_{\infty h} = C_{\infty v} \times C_i$ contain the following symmetry operations:

$$\begin{aligned} C_{\infty v} &= \{R^{(z)}(\varphi),\ \sigma^{(\varphi)}\}\ , \quad 0 \le \varphi < 2\pi\ , \\ D_{\infty h} &= \{R_z(\varphi),\ \sigma^{(\varphi)},\ C_2^{(\varphi)},\ S_z(\varphi), I\}\ , \quad 0 \le \varphi < 2\pi\ . \end{aligned} \tag{8-29}$$

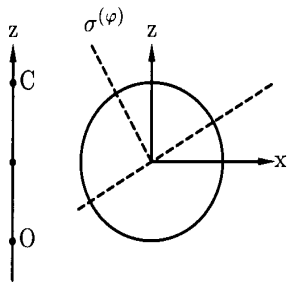


Fig. 8.2-7. The molecule CO with $\mathcal{C}_{\infty v}$ symmetry.

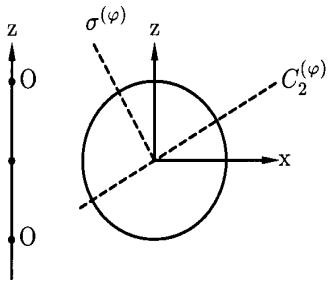


Fig. 8.2-8. The molecule O_2 with $D_{\infty h}$ symmetry.

The subgroup chains for the 32 crystal point groups are shown in Fig. 8.2-9 (taken from Koster 1963).

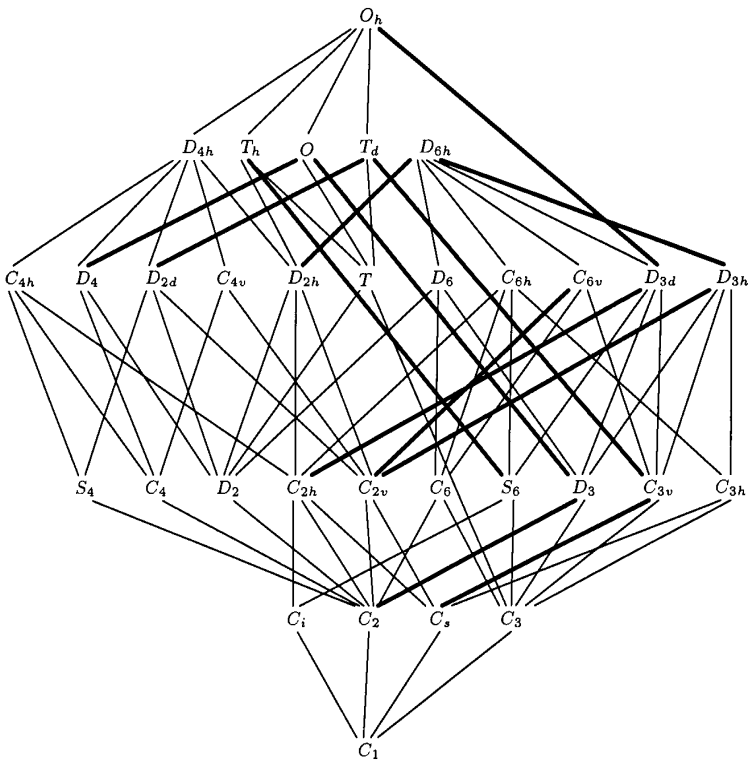


Fig. 8.2-9. Subgroup chains of the 32 point groups.
A heavy line indicates that the subgroup is not invariant.

Ex. 8.1. Show that $S_{2n} = \mathcal{C}_n \times \mathcal{C}_i$ for odd n, and $S_{2n} \sim \mathcal{C}_{2n}$ for even n.

Ex. 8.2. Show that $\mathcal{C}_{nh} \sim \mathcal{C}_{2n}$ for odd n, and $\mathcal{C}_{nh} = \mathcal{C}_n \times \mathcal{C}_i$ for even n.

Ex. 8.3. Show that $D_{nd} = S_{2n} \wedge \mathcal{C}_{2x}$ and $D_{nh} = \mathcal{C}_{nh} \wedge \mathcal{C}_{2x}$.

Ex. 8.4. Using the results of Ex. 8.1 and 8.3 show that $D_{nd} = D_n \times \mathcal{C}_i$ for odd n and $D_{nd} \sim D_{2n}$ for even n.

Ex. 8.5. Using the results of Ex. 8.2 and 8.3 show that $D_{nh} \sim D_{2n}$ for odd n and $D_{nh} = D_n \times C_i$ for even n.

Ex. 8.6. Check that the point groups in (8-27) obey the requirement for semi-direct product groups

8.3. Character Tables of Point Groups

8.3.1. The conventional labelling for point group irreps (Mulliken Notation)

1. Use A or B to denote one-dimensional irreps; E, two-dimensional irreps; T or F, three-dimensional irreps.
2. $A(B)$ are used to denote irreps with character $\chi(C_n) = 1(-1)$.
3. A_1 or B_1 are used to denote irreps with $\chi(C_2) = 1$ or $\chi(\sigma_v) = 1$, where C_2 is a 2-fold. axis perpendicular to the principal axis. A_2 or B_2 denote irreps with $\chi(C_2) = -1$ or $\chi(\sigma_v) = -1$.
4. A', B', E' and T' are associated with $\chi(\sigma_h) = 1$, while A'', B'', E'' and T'' are associated with $\chi(\sigma_h) = 1$.
5. A_g, B_g, E_g and T_g are associated with $\chi(I) = 1$, while A_u, B_u, E_u and T_u are associated with $\chi(I) = -1$.

8.3.2. Character tables of point groups

The character tables of point groups are all known and are listed in many books (Koster 1963, Bradley & Cracknell 1972, Butler 1981). The character tables for commonly used point groups are listed in Table 8.3-1 to Table 8.3-9. The last row of Table 8.3-1 and the last columns in the remaining tables list the *types* a,b,c of the irreps introduced in Sec. 3.12.

A novel point in the tabulation in Table 8.3-1 to Table 8.3-9 is that the characters for both s-v and d-v reps of point groups are listed in a compact form. For s-v reps, one just ignores the tilded classes. Only the character tables of the proper cubic groups and icosahedral group are given. The character $\chi^{\Gamma\pm}$ of the improper point groups $G_h = G \times C_i$ are easily obtainable from the character χ^{Γ} of G by

$$\begin{aligned} \chi^{\Gamma\pm}(R) &= \chi^{\Gamma}(R), \quad \text{for proper rotation;} \\ \chi^{\Gamma\pm}(R) &= \pm\chi^{\Gamma}(R), \quad \text{for improper rotation,} \end{aligned} \tag{8-29}$$

where $\Gamma_+ \equiv \Gamma_g, \Gamma_- \equiv \Gamma_u$.

Ex. 8.7. Using (3-250) check the types of irreps of the groups D_3 and T.

Ex. 8.8. Construct the character table of O_h.

8.4. The CSCO-I and CSCO-II of Point Groups

The CSCO-I and CSCO-II given in this section are valid for both s-v and d-v reps, though the discussion of the d-v reps is postponed to Sec. 8.11 for pedagogical reason.

8.4.1. The CSCO-I of point groups

The CSCO of the cyclic group C_n and its eigenvalue are:

$$C = C_{nz}, \quad \lambda_\mu = \exp(-2\pi\mu i/n), \quad \mu = 0, \pm\tfrac{1}{2}, \pm 1, \cdots, \pm\tfrac{n-1}{2}, \tfrac{n}{2}\ . \tag{8-30a}$$

The CSCO of S_{2n} (even n) and C_{nh} (odd n) and their eigenvalues are found (see Sec. 8.12) as

$$S_{2n}: \quad C = S_{2n,z}, \quad \lambda_\mu = (-1)^{2\mu}\omega^{(n+1)\mu}, \tag{8-30b}$$

Table 8.3-1a. Characters of C_n (odd n). $\chi^{\mu}(C_{nz}^{k})=\exp(-2k\mu\pi i/n)$. The last row gives the type a,b,c of irreps defined in Theorem 3.32.

	s–v				d–v			
irreps	0	±1	$\cdots$	$\pm\frac{n-1}{2}$	$\pm\frac{1}{2}$	$\cdots$	$\pm\frac{n-2}{2}$	$\frac{n}{2}$
types	a	c	$\cdots$	c	c	$\cdots$	c	a

Table 8.3-1b. Characters of C_{2n}, S_{2n} (even n) and C_{nh} (odd n). $\chi^{\mu}(C_{2n,z}^{k})=\omega^{k\mu}$, $\chi^{\mu}(S_{2n,z}^{k})=(-1)^{2k\mu}\omega^{(n+1)k\mu}$, $\chi^{\mu}(S_{nz}^{k})=(-1)^{2k\mu}\omega^{(n+2)k\mu}$, $\omega=\exp(-\frac{\pi}{n}i)$.

	s–v					d–v		
irreps	0	±1	$\cdots$	$\pm(n-1)$	n	$\pm\frac{1}{2}$	$\cdots$	$\pm(n-\frac{1}{2})$
types	a	c	$\cdots$	c	a	c	$\cdots$	c

$$C_{nh}: \quad C=S_{nz}, \quad \lambda_{\mu}=(-1)^{2\mu}\omega^{(n+2)\mu}, \tag{8-30c}$$

where $\omega=\exp(-\pi\mu i/n)$, $\mu=0,\pm\frac{1}{2},\pm1,\pm\frac{3}{2},\cdots,\pm(n-\frac{1}{2}),n$.

The irreps of C_n, S_{2n} and C_{nh} can be labelled by the quantum number μ, with integer (half integer) representing the s–v (d–v) reps. The correspondence between the Koster notation Γ_i and μ is given in p. 192-194 of Butler (1981).

For non-cyclic point groups, we can use the method of Sec. 3.12 and Table 8.3 to find their CSCO's quite easily. The CSCO of the dihedral groups D_n consist of two class operators

$$C_{D_{\text{even}}}=(2C_{nz},\tfrac{n}{2}C_2), \qquad C_{D_{\text{odd}}}=(2C_{nz},nC_2), \tag{8-30d}$$

for even and odd n respectively. For one–dimensional irreps it is more convenient to use the set of operators (C_{nz},C_{2x}) as the CSCO, whose eigenvalue (ρ,ν) uniquely labels the one–dimensional irreps, as shown in Tables 8.4-1 and 8.4-2.

The CSCO's of the groups T,O,I consist of only a single class operator each,

$$C_T=C_{31}^{+}+C_{32}^{+}+C_{33}^{+}+C_{43}^{+}, \tag{8-30e}$$

$$C_O=C_{4x}^{+}+C_{4y}^{+}+C_{4z}^{+}+C_{4x}^{-}+C_{4y}^{-}+C_{4z}^{-}, \tag{8-30f}$$

$$C_I=\sum_{i=1}^{6}(C_{5i}^{+}+C_{5i}^{-}). \tag{8-30g}$$

The correspondence between their eigenvalues and the irrep labels is shown in Tables 8.3-7, 8.3-8 and 8.3-9.

The CSCO's of the improper point groups D_{nh},T_h,O_h,I_h are easily found using (3-37); namely they are $(C,\hat{I})$, where C are the CSCO's of the corresponding proper point groups.

8.4.2. The CSCO–II of point groups

According to Theorem 3.21, if we find a canonical subgroup chain $G\supset G(s)$, than $(C,C(s))$ will be the CSCO–II of G. Therefore to find the CSCO–II's of a point group, we only need to list its possible canonical group chains. The problem of which canonical subgroup chain should be used depends on the practical problem concerned. If the Hamiltonian of a system can be written as $H=aH_0+bH_1+cH_3$, and suppose $[H_i,G_i]=0$ and $a\gg b\gg c$, than it is convenient

Table 8.3-2. Characters of D_2 . The first and second columns are Koster, Mulliken (or modified Mulliken) notations, respectively. For one–dimensional irreps, the character χ_i^ν is equal to the eigenvalue λ_i^ν of any operator in the class i. The last column gives the type a,b,c of the irrep as in Theorem 3.32.

	C_{2v}	e	$(\sigma_x, \tilde{\sigma}_x)$	$(\sigma_y, \tilde{\sigma}_y)$	$(C_{2z}, \tilde{C}_{2z})$	basis vectors	
	D_2	e	$(C_{2x}, \tilde{C}_{2x})$	$(C_{2y}, \tilde{C}_{2y})$	$(C_{2z}, \tilde{C}_{2z})$	of D_2	type
Γ_1	A_1	1	1	1	1		a
Γ_2	B_1	1	−1	−1	1	z	a
Γ_3	B_2	1	−1	1	−1	y	a
Γ_4	B_3	1	1	−1	−1	x	a
Γ_5	$E_{1/2}$	2	0	0	0		b

Table 8.3-3. Characters of D_3.

	C_{3v}	e	$2C_{3z}$	3σ	
	D_3	e	$2C_{3z}$	$3C_2$	type
Γ_1	A_1	1	1	1	a
Γ_2	A_2	1	1	−1	a
Γ_3	E	2	−1	0	a
Γ_5	$A_{3/2}$	1	−1	$-i$	c
Γ_6	$A_{-3/2}$	1	−1	i	c
Γ_4	$E_{1/2}$	2	1	0	b

Table 8.3-4. Characters of D_4. $2C_2 = (C_{2x}, C_{2y})$, $2\sigma = (\sigma_x, \sigma_y)$.

	D_{2d}	e	$2S_{4z}$	$(C_{2z}, \tilde{C}_{2z})$	$(2C_2, 2\tilde{C}_2)$	$(2\sigma, 2\tilde{\sigma})$	
	C_{4v}	e	$2C_{4z}$	$(C_{2z}, \tilde{C}_{2z})$	$(2\sigma, 2\tilde{\sigma})$	$(2\sigma', 2\tilde{\sigma}')$	
	D_4	e	$2C_{4z}$	$(C_{2z}, \tilde{C}_{2z})$	$(2C_2, 2\tilde{C}_2)$	$(2C_2', 2\tilde{C}_2')$	type
Γ_1	A_1	1	1	1	1	1	a
Γ_2	A_2	1	1	1	−1	−1	a
Γ_3	B_1	1	−1	1	1	−1	a
Γ_4	B_2	1	−1	1	−1	1	a
Γ_5	E	2	0	−2	0	0	a
Γ_6	$E_{1/2}$	2	$\sqrt{2}$	0	0	0	b
Γ_7	$E_{1/2}$	2	$-\sqrt{2}$	0	0	0	b

Table 8.3-5. Characters of D_5. $c_\mu = \cos\frac{2\mu\pi}{5}$, $c_1 = \frac{\sqrt{5}-1}{4}$, $c_2 = -\frac{\sqrt{5}+1}{4}$.

C_{5v}	e	$2C_{5z}$	$2C_{5z}^2$	5σ	
D_5	e	$2C_{5z}$	$2C_{5z}^2$	$5C_2$	type
A_1	1	1	1	1	a
A_2	1	1	1	−1	a
E_1	2	$2c_1$	$2c_2$	0	a
E_2	2	$2c_2$	$2c_1$	0	a
$A_{5/2}$	1	−1	1	$-i$	c
$A_{-5/2}$	1	−1	1	i	c
$E_{1/2}$	2	$-2c_2$	$2c_1$	0	b
$E_{3/2}$	2	$-2c_1$	$2c_2$	0	b

Table 8.3-6. Characters of D_6 . $2C_2 = (\ C_{2x},\ C_{22},\ C_{24}\ )$, $2\sigma=(\sigma_x,\sigma_2,\sigma_4)$.

	D_{3h}	e	$2S_{3z}$	$2C_{3z}$	$(\sigma_z,\tilde{\sigma}_z)$	$(3C_2,3\tilde{C}_2)$	$(3\sigma,3\tilde{\sigma})$	
	C_{6v}	e	$2C_{6z}$	$2C_{3z}$	$(C_{2z},\tilde{C}_{2z})$	$(3\sigma,3\tilde{\sigma})$	$(3\sigma',3\tilde{\sigma}')$	
	D_6	e	$2C_{6z}$	$2C_{3z}$	$(C_{2z},\tilde{C}_{2z})$	$(3C_2,3\tilde{C}_2)$	$(3C_2',3\tilde{C}_2')$	type
Γ_1	A_1	1	1	1	1	1	1	a
Γ_2	A_2	1	1	1	1	−1	−1	a
Γ_3	B_1	1	−1	1	−1	1	−1	a
Γ_4	B_2	1	−1	1	−1	−1	1	a
Γ_5	E_1	2	1	−1	−2	0	0	a
Γ_6	E_1	2	−1	−1	2	0	0	a
Γ_7	$E_{1/2}$	2	$\sqrt{3}$	1	0	0	0	b
Γ_9	$E_{3/2}$	2	0	−2	0	0	0	b
Γ_8	$E_{3/2}$	2	$-\sqrt{3}$	1	0	0	0	b

Table 8.3-7. Characters and eigenvalues λ of the CSCO of T . The CSCO of T is $C = C_{31}^{+} + C_{32}^{+} + C_{33}^{+} + C_{43}^{+}$, $\epsilon = \exp(-\frac{2\pi i}{3})$.

	T	λ	e	$4C_3$	$4C_3^{-1}$	$(3C_2,3\tilde{C}_2)$	type
Γ_1	A_0	4	1	1	1	1	a
Γ_2	A_1	4ϵ	1	ϵ	ϵ^2	1	c
Γ_3	A_{-1}	$4\epsilon^*$	1	ϵ^2	ϵ	1	c
Γ_4	F	0	3	0	0	−1	a
Γ_5	$E_{1/2}$	2	2	1	1	0	b
Γ_6	$E_{3/2}$	2ϵ	2	ϵ	ϵ^2	0	c
Γ_7	$E_{-3/2}$	$2\epsilon^*$	2	ϵ^2	ϵ	0	c

Table 8.3-8. Characters and eigenvalues λ of the CSCO of O. The CSCO of O is $C = C_{4x}^{+} + C_{4y}^{+} + C_{4z}^{+} + C_{4x}^{-} + C_{4y}^{-} + C_{4z}^{-}$.

	T_d	λ	e	$8C_3$	6σ	$(3C_2,3\tilde{C}_2)$	$(6\sigma,6\tilde{\sigma}_2)$	
	O	λ	e	$8C_3$	$6C_4$	$(3C_2,3\tilde{C}_2)$	$(6C_2,6\tilde{C}_2)$	type
Γ_1	A_1	6	1	1	1	1	1	a
Γ_2	A_{-1}	−6	1	1	−1	1	−1	a
Γ_3	E	0	2	−1	0	2	0	a
Γ_4	F_1	2	3	0	1	−1	−1	a
Γ_5	F_{-1}	−2	3	0	−1	−1	1	a
Γ_6	$E_{1/2}$	$3\sqrt{2}$	2	1	$\sqrt{2}$	0	0	b
Γ_7	$E_{3/2}$	$-3\sqrt{2}$	2	1	$-\sqrt{2}$	0	0	b
Γ_8	$G_{3/2}$	0	4	−1	0	0	0	b

Table 8.3-9. Characters and eigenvalues λ of the CSCO of I. The CSCO of I is $C = \sum_{i=1}^{6} \left(C_{5i}^{+} + C_{5i}^{-} \right)$, $c_\mu = \cos \frac{2\mu\pi}{5}, c_1 = \frac{\sqrt{5}-1}{4}$, $c_2 = -\frac{\sqrt{5}+1}{4}$.

I	λ	e	$12C_5$	$12C_5^2$	$20C_3$	$(15C_2, 15\tilde{C}_2)$	type
A_1	12	1	1	1	1	1	a
F_1	$-8c_2$	3	$-2c_2$	$-2c_1$	0	-1	a
F_2	$-8c_1$	3	$-2c_1$	$-2c_2$	0	-1	a
G	-3	4	-1	-1	1	0	a
H	0	5	0	0	-1	1	a
$E_{1/2}$	$-12c_2$	2	$-2c_2$	$2c_1$	1	0	b
$E_{3/2}$	$-12c_1$	2	$-2c_1$	$2c_2$	1	0	b
$G_{3/2}$	3	4	1	-1	-1	0	b
$I_{5/2}$	-2	6	-1	1	0	0	b

Table 8.4-1. Eigenvalues of the CSCO of D_n (even n). $\mu = 1, 2, \cdots, \frac{n}{2}-1$ for s-v reps, $\mu = \frac{1}{2}, \frac{3}{2}, \cdots, \frac{n-1}{2}$ for d-v reps. ρ and ν are eigenvalues of C_{nz} and C_{2x}, respectively.

	A_1	A_2	B_1	B_2	E_μ
$(2C_{nz}, \frac{n}{2}C_2)$	$(2, \frac{n}{2})$	$(2, -\frac{n}{2})$	$(-2, \frac{n}{2})$	$(-2, -\frac{n}{2})$	$(2\cos\frac{2\pi\mu}{n}, 0)$
(ρ, ν)	$(1, 1)$	$(1, -1)$	$(-1, 1)$	$(-1, -1)$	

Table 8.4-2. Eigenvalues of the CSCO of D_n (odd n). The irreps $A_{\pm\frac{n}{2}}$ are double-valued. $\mu = 1, 2, \cdots, \frac{n-1}{2}$ for s-v, $\mu = \frac{1}{2}, \frac{3}{2}, \cdots, \frac{n}{2}-1$ for d-v.

	A_1	A_2	$A_{\frac{n}{2}}$	$A_{-\frac{n}{2}}$	E_μ
$(2C_{nz}, nC_2)$	$(2, n)$	$(2, -n)$	$(-2, -ni)$	$(-2, ni)$	$(2\cos\frac{2\pi\mu}{n}, 0)$
(ρ, ν)	$(1, 1)$	$(1, -1)$	$(-1, -i)$	$(-1, i)$	

to use the irreducible bases symmetry adapted to $G_0 \supset G_1 \supset G_2$, since they are the eigenvectors of the perturbed Hamiltonian to the first order of approximation. If a system has the perfect symmetry G, than we can use any canonical subgroup chain of G.

The canonical group chains for dihedral groups are

$$D_n \supset C_n, \quad D_n \supset \mathcal{C}_{2x},$$

$$C_{nv} \supset C_n, \quad C_{nv} \supset \mathcal{C}_{sx},$$

$$D_{nd} \supset S_{2n}, \quad D_{nd} \supset \mathcal{C}_{2x},$$

$$D_{nh} \supset \mathcal{C}_{nh}, \quad D_{nh} \supset \mathcal{C}_{2x}.$$

The canonical subgroup chains for the cubic groups and icosahedral groups can be found from the branching rule (or subduction rule) tables on pages 214–216 of Butler (1981).

1. The group T:

	s–v	s–v & d–v	d–v
1	$T \supset D_2$		$T \supset \mathcal{C}_{2z}$
2		$T \supset \mathcal{C}_3$	

2. The group T_d ($\mathcal{C}_{sa} = \{e, \sigma_{da}\}$):

	s–v	s–v & d–v	d–v
1		$T_d \supset D_{2d} \supset \mathcal{C}_{2x}$	
2		$T_d \supset D_{2d} \supset \mathcal{C}_{sa}$	
3		$T_d \supset C_{3v} \supset \mathcal{C}_3$	
4		$T_d \supset C_{3v} \supset \mathcal{C}_{sb}$	
5		$T_d \supset T \supset \mathcal{C}_3$	
6	$T_d \supset D_{2d} \supset D_2$		$T_d \supset T \supset \mathcal{C}_{2x}$
7	$T_d \supset D_{2d} \supset C'_{2v}$		

3. The group O ($D'_2 = \{e, C_{2c}, C_{2e}, C_{2y}\}$):

	s–v	s–v & d–v	d–v
1		$O \supset D_4 \supset \mathcal{C}_{2x}$	
2		$O \supset D_3 \supset \mathcal{C}_{2b}$	
3		$O \supset D_3 \supset \mathcal{C}_3$	
4		$O \supset T \supset \mathcal{C}_3$	
5		$O \supset \mathcal{C}_{4z}$	
6	$O \supset D_4 \supset D_2$		$O \supset T \supset \mathcal{C}_{2x}$
7	$O \supset T \supset D_2$		
8	$O \supset D'_2$		

4. The group O_h:

	s–v	s–v & d–v	d–v
1		$O_h \supset D_{2d} \supset \mathcal{C}_{sa}$	
2		$O_h \supset D_{2d} \supset \mathcal{C}_{2x}$	
3		$O_h \supset C_{4v} \supset \mathcal{C}_{sx}$	
4		$O_h \supset C_{3v} \supset \mathcal{C}_3$	
5	$O_h \supset D_{2d} \supset D_2$		$O_h \supset C_{3v} \supset \mathcal{C}_{sb}$
6	$O_h \supset C_{4v} \supset C_{2v}$		

8.4.3. The codes for point groups

The irreducible matrices of any point group symmetry adapted to a canonical subgroup chain can be found using the EFM. Suppose that the projection operator $P^{(\lambda)\bar{\mu},\bar{\rho}}_{\mu,\rho}$ is symmetry adapted to a canonical subgroup chain $G \supset H \supset K$, where K is an Abelian group. Let the CSCO and their eigenvalues (effectively the irrep labels) of the various groups be denoted by:

$$\begin{array}{cccc} & G \supset & H \supset & K \\ \text{CSCO} & C & C_H & C_K \\ \text{irrep} & \lambda & \mu & \rho \end{array}$$

The operator $P^{(\lambda)\bar{\mu},\bar{\rho}}_{\mu,\rho}$ is necessarily a simultaneous eigenvector of the CSCO-III, (C, C_H, C_K, $\bar{C}_H$, $\bar{C}_K$),

$$\begin{pmatrix} C \\ C_H \\ C_K \\ \bar{C}_H \\ \bar{C}_K \end{pmatrix} P^{(\lambda)\bar{\mu},\bar{\rho}}_{\mu,\rho} = \begin{pmatrix} \lambda \\ \mu \\ \rho \\ \bar{\mu} \\ \bar{\rho} \end{pmatrix} P^{(\lambda)\bar{\mu},\bar{\rho}}_{\mu,\rho}. \tag{8-31}$$

Now the irrep labels (μ, ρ) of the subgroups serve as the component index of the irrep λ.

With given group table, by solving the eigenvalue equations (8-31) numerically, we can find the irreducible matrices of G. A program for point groups is available (Chen & Ping, 1999) by which the characters, irreducible matrices and Clebsch-Gordan coefficients of any crystallographic point group G adapted to any canonical group chain $G \supset H \supset K$ can be calculated *ab initio* for both single-valued and double-valued representations and tabulated with exact values in the form of $\sqrt{\frac{p}{q}}\exp(i\pi\sqrt{\frac{m}{n}})$ or $\sqrt{\frac{p}{q}}\exp(i\cos^{-1}\sqrt{\frac{m}{n}})$.

Alternatively, if we regarded the eigenvalues $\lambda, \mu, \rho, \bar{\mu}, \bar{\rho}$ as parameters, and find the eigenvectors $P^{(\lambda)\bar{\mu},\bar{\rho}}_{\mu,\rho}$ as a functions of these parameters, then we find algebraic instead of numerical solutions. The advantages of the algebraic solutions over the numerical solutions are obvious in that the lengthy tabulations will become redundant. Algebraic solutions for all point groups in various subgroup chains have been found (Chen & Fan 1998, Fan & Chen 1999, Fan, Chen & Draayer 1999). Due to space limitations, we only discuss the algebraic solutions for the dihedral groups D_n and for the cubic groups T and O.

Another program RACAH v3.1 (Ross *et al.* 1996) follows the approach of Butler (1981) and of Searle and Butler (1988), with which one can calculate the $3jm$, $6j$ symbols and the symmetry adapted functions (see Sec. 8.5.6) of point groups (and other groups). Significant progress has since been made on developing that software into a tool for the recursive calculation of arbitrary Hamiltonian.

8.4.4. The point group tables

Many tables for the point groups exist, for examples, in Koster et al (1963), McWeeny (1963), Bradley & Cracknell (1972), and Butler (1981). The most extensive tables are in a recently published book by Altmann & Herzig (1994). That book contains diagrams and Euler angles of the group elements, group tables, characters, irreducible matrices, symmetry adapted functions (defined in Sec. 8.5.7), subduction rules, the CG series and CG coefficients of 75 point groups, including the cyclic groups C_n, S_{2n}, C_{nh}, the dihedral groups $D_n, C_{nv}, D_{nd}, D_{nh}$, $n = 2, 3, \cdots, 10$, tetrahedral, octahedral and icosahedral groups.

8.5. Algebraic Solutions for the Dihedral Groups D_n

Numerical solutions for the point groups, especially for the dihedral groups, are well known. The shortcomings of numerical solutions are obvious, for example for practical calculations one has needed to look at various tables, which may not be readily available, and are subject to printing or other errors. Another significant difficulty with the bulky tabulated material (for example Altmann and Herzig 1994), is that regularities are hard to find. It is highly desirable therefore to obtain analytic or algebraic solutions for all point groups, just as we have for the rotation group. Significant progress has been made in this direction (Fan, Chen & Draayer 1999, and references therein). In this section we introduce the algebraic solutions for the dihedral groups.

8.5.1. Factorization lemma for the projection operators

It is known that the projection operator for a direct product group $H \times K$ is a product of the projection operators of H and K. Now we are going to generalizing this factorization to a group G which is a semi-direct product of two Abelian groups H and K, $G = H \wedge K$. Suppose that the $G \supset H$ and $G \supset K$ irreducible bases are ψ_ρ^λ and φ_ν^λ, respectively. The $G \supset H, \bar{G} \supset \bar{H}$ projection operator and the $G \supset H, \bar{G} \supset \bar{K}$ generalized projection operator (see Eq. (3-242a)) are denoted by

$$\mathcal{P}_{\rho,\bar{\rho}}^{(\lambda)} = \frac{h_\lambda}{|G|} \sum_{a=1}^{|G|} D_{\rho\bar{\rho}}^{(\lambda)}(R_a)^* R_a, \tag{8-32a}$$

$$\mathcal{P}_{\rho,\nu}^{(\lambda)} = \frac{h_\lambda}{|G|} \sum_{a=1}^{|G|} \mathcal{D}_{\rho\nu}^{(\lambda)}(R_a)^* R_a, \tag{8-32b}$$

where $\mathcal{D}_{\rho\nu}^{(\lambda)}$ is the generalized irreducible matrix element,

$$\mathcal{D}_{\rho\nu}^{(\lambda)}(R_a) = \langle \psi_\rho^\lambda | R_a | \varphi_\nu^\lambda \rangle. \tag{8-32c}$$

Let $C(s)$ and $C(s')$ be the CSCO of H and K, we have

$$\big(C, C(s), \bar{C}(s)\big)\mathcal{P}_{\rho,\bar{\rho}}^{(\lambda)} = (\lambda, \rho, \bar{\rho})\mathcal{P}_{\rho,\bar{\rho}}^{(\lambda)}, \tag{8-32d}$$

$$\big(C, C(s), \bar{C}(s')\big)\mathcal{P}_{\rho,\nu}^{(\lambda)} = (\lambda, \rho, \nu)\mathcal{P}_{\rho,\nu}^{(\lambda)}. \tag{8-32e}$$

The generalized projection operator satisfies

$$\mathcal{P}_{\rho,\nu}^{(\lambda)}\mathcal{P}_{\nu',\rho'}^{(\lambda')} = \delta_{\lambda\lambda'}\delta_{\nu\nu'}\mathcal{P}_{\rho,\rho'}^{(\lambda)}, \quad (\mathcal{P}_{\rho,\nu}^{(\lambda)})^\dagger = \mathcal{P}_{\nu,\rho}^{(\lambda)}. \tag{8-32f}$$

Since the numerical factor $\frac{h_\lambda}{|G|}$ in the projection operator $\mathcal{P}_{\rho,\nu}^{(\lambda)}$ or $\mathcal{P}_{\rho,\bar{\rho}}^{(\lambda)}$ is unimportant in applications except in the case of reading out the irreducible matrices from them according to (8-32), for the sake of clarity we are sloppy about the numerical factor of the projection operator, but careful about its phase.

Lemma : If H and K are two Abelian groups with the projection operators P^ρ and $\wp^\nu$, respectively, then the projection operators of the semi-direct product group $G = H \wedge K$ for four possible classifications are factored in the following way:

$$G \supset H, \bar{G} \supset \bar{K}: \ \mathcal{P}_{\rho,\nu}^{(\lambda)} = P^\rho \wp^\nu, \tag{8-33a}$$

$$G \supset K, \bar{G} \supset \bar{H}: \ \mathcal{P}_{\nu,\rho}^{(\lambda)} = \wp^\nu P^\rho, \tag{8-33b}$$

$$G \supset H, \bar{G} \supset \bar{H}: \ \mathcal{P}_{\rho,\rho'}^{(\lambda)} = P^\rho \wp^\nu P^{\rho'}, \tag{8-33c}$$

$$G \supset K, \bar{G} \supset \bar{K}: \ \mathcal{P}_{\nu,\nu'}^{(\lambda)} = \wp^\nu P^\rho \wp^{\nu'}. \tag{8-33d}$$

Proof: Since P^ρ and $\wp^\nu$ are the projection operator of H and K, respectively, they are eigenvectors of the CSCO's of H and K,

$$C(s)P^\rho = \rho P^\rho,\ C(s')\wp^\nu = \nu\wp^\nu. \tag{8-34a}$$

Since $C(s)$ and $C(s')$ are the CSCO's of H and K, they have $|H|$ and $|K|$ distinct eigenvalues, ρ and ν, respectively. The operators $C(s)$ and $C(s')$ can be easily found, for example, the generators of the Abelian groups H and K can be chosen as $C(s)$ and $C(s')$, respectively. Now let us derive the eigenvalue equations satisfied by $P^\rho\wp^\nu$. Using (3-129), (8-34a) and the commutation of $\wp^\nu$ with $C(s')$, we can show that $P^\rho\wp^\nu$ is a common eigenvector of $C(s)$ and $\bar{C}(s')$,

$$\begin{pmatrix} C(s) \\ \bar{C}(s') \end{pmatrix} P^\rho\wp^\nu = \begin{pmatrix} C(s)P^\rho\wp^\nu \\ P^\rho\wp^\nu C(s') \end{pmatrix} = \begin{pmatrix} \rho \\ \nu \end{pmatrix} P^\rho\wp^\nu. \tag{8-34b}$$

It is to be noted that the set of operators $(C(s), \bar{C}(s'))$ has $|G| = |H| \times |K|$ sets of eigenvalues (ρ, ν) and for a given (ρ, ν) we have a unique eigenvector $P^\rho\wp^\nu$. In other words, $(C(s), \bar{C}(s'))$ is already a CSCO-III of G, and C is redundant. This can also be shown in the following way. Since C commutes with $C(s)$ and $\bar{C}(s')$, $CP^\rho\wp^\nu$ remains to be an eigenvector of $(C(s), \bar{C}(s'))$ with the same eigenvalue set (ρ, ν). Due to the uniqueness of the solution in the eigenvalue equation (8-34b), $CP^\rho\wp^\nu$ is necessarily proportional to $P^\rho\wp^\nu$, that is

$$CP^\rho\wp^\nu = \lambda P^\rho\wp^\nu. \tag{8-34c}$$

Thus $P^\rho\wp^\nu$ is a simultaneous eigenvector of $(C, C(s), \bar{C}(s'))$. Comparing (8-34b,c) with (8-32e) we know that $P^\rho\wp^\nu$ is necessarily the projection operator $\mathcal{P}^{(\lambda)}_{\rho,\nu}$ of G. It shows that for a group G which is a semi-direct product of two Abelian groups, the operator C of G is redundant for determining the projection operator of G. Actually, according to Theorem 2.2 (Dirac's Theorem), C is necessarily a function of $C(s)$ and $\bar{C}(s')$, and thus λ is a function of ρ and ν.

Eq. (8-33b) can be proved in the same way, while Eq. (8-33c) and (8-33d) can be derived from Eq. (8-32f). **QED**

Remark 1: Comparing (8-33a,b) with (8-33c,d) it is seen that the factorization of the generalized projection operators is simpler than for the conventional projection operators.

Remark 2: The projection operators $\mathcal{P}^{(\lambda)}_{\rho,\rho'} = P^\rho\wp^\nu P^{\rho'}$ with different values of ν differ at most by a ν-dependent factor so long the irrep λ of G can be induced from ν. Therefore to obtain $\mathcal{P}^{(\lambda)}_{\rho,\rho'}$ through using $P^\rho\wp^\nu P^{\rho'}$ we can choose any value ν which is compatible with λ. Similar remarks apply to $\mathcal{P}^{(\lambda)}_{\nu,\nu'} = \wp^\nu P^\rho\wp^{\nu'}$.

Remark 3: We have a unified expression $P^\rho\wp^\nu$ for the $G \supset H$ generalized projection operators for both one-dimensional and multi-dimensional irreps, but with the essential difference that the factors P^ρ and $\wp^\nu$ are interchangeable for one-dimensional irreps but not for multi-dimensional irreps. In other words, for one-dimensional irreps the generators of both the subgroups H and K have definite values ρ and ν, respectively, while for multi-dimensional irreps only the generator of H (not K) has the definite value ρ. Therefore we can use (ρ, ν) or $A_{\rho\nu}$ as labels for the one-dimensional irreps, and write

$$\mathcal{P}^{A_{\rho\nu}} = P^\rho\wp^\nu = \wp^\nu P^\rho. \tag{8-35a}$$

Remark 4: The factorization $\mathcal{P}^{(\lambda)}_{\rho,\rho'} = P^\rho\wp^\nu P^{\rho'}$ is to be compared with the factorization in (3-241),

$$\mathcal{P}^{(\lambda)}_{\rho,\rho'} = \mathcal{P}^\lambda P^\rho R_a P^{\rho'}, \tag{8-35b}$$

where $\mathcal{P}^\lambda$ is the projection operator of the non–Abelian group G, and R_a is an appropriate element of G which can be chosen freely so long as $P^\rho R_a P^{\rho'} \neq 0$. Evidently, the factorization (8-33c) is much simpler than the factorizations in (8-35b), since the latter involves the projection operator $\mathcal{P}^\lambda$ of the non–Abelian group G.

8.5.2. $D_n \supset \mathcal{C}_{2x}$ generalized projection operators of D_n

The group D_n has $2n$ elements

$$D_n = C_n \wedge \mathcal{C}_{2x} = \{C_{nz}^k, C_{2k} : k = 0, 1, \cdots, n-1\},$$
$$C_{nz} = \exp(-\tfrac{2\pi J_z i}{n}). \tag{8-36a}$$

The k–th two–fold axis C_{2k} is generated from $C_{20} = C_{2x}$ by

$$C_{2k} = C_{nz}^k C_{20}. \tag{8-36b}$$

In other words, the axis of the C_{2k} is obtained by rotating that of C_{2x} about the z–axis through angle $\frac{k\pi}{n}$ anti–clock wise. The two–fold axes of D_2–D_6 are shown in Fig. 8.2-1.

The eigenvalue of C_{nz} is denoted by

$$\rho \equiv \rho_\mu = \exp(-\tfrac{2\pi\mu}{n} i), \tag{8-36c}$$

with the values of μ given below:

$$\mu = 0, \pm 1, \pm 2.... \begin{cases} \pm\frac{n-1}{2}, & n = \text{odd}, \\ \pm\frac{n-2}{2}, \frac{n}{2}, & n = \text{even}. \end{cases} \tag{8-36d}$$

It is readily seen that C_{nz} is a CSCO of C_n, and its eigenvalue ρ, or equivalently μ, can be used to label irreps of C_n. Similarly the CSCO of $\mathcal{C}_{2x}$ is C_{2x} whose eigenvalue is denoted by $\nu = \pm 1$.

Now we apply the factorization lemma to the dihedral groups D_n with $H = C_n$, $K = \mathcal{C}_{2x}$, $C(s) = C_{nz}, \bar{C}(s') = C_{2x}$.

One–dimensional projection operators

The unnormalized projection operator of C_n is

$$P^\mu \equiv P^{\rho_\mu} = \sum_{k=0}^{n-1} (\rho_\mu^*)^k (C_{nz})^k \ . \tag{8-37a}$$

The projection operator of the group $\mathcal{C}_{2x} = \{e, C_{2x}\}$ is

$$\wp^\nu = (1 + \nu^* C_{2x}), \ \nu = \pm 1. \tag{8-37b}$$

According to (8-35a), the one–dimensional projection operators of D_n can be written down directly,

$$\mathcal{P}^{A_{\rho\nu}} = \wp^\nu P^\rho = P^\rho \wp^\nu = P^\rho (1 + \nu^* C_{2x}), \tag{8-37c}$$

$$\rho = \begin{cases} 1, \ \nu = \pm 1, \ n = \text{even or odd}, \\ -1, \ \nu = \pm 1, \ n = \text{even}; \end{cases} \tag{8-37d}$$

As is seen, using the eigenvalues (ρ, ν) as irrep label is crucial for getting a simple algebraic expression for the one–dimensional projection operators. Table 8.4 gives the switch board between the notation $A_{\rho\nu}$ and the Mulliken notation.

Next we come to the projection operators for multi–dimensional irreps, which depend on the group chain.

The $D_n \supset C_{2x}$ generalized projection operators

Now ρ is complex, since ρ real corresponds to one–dimensional irreps. According to (8-33b), the $D_n \supset C_{2x}$ and $\bar{D}_n \supset \bar{C}_n$ projection operator is $\mathcal{P}^{(\lambda)}_{\nu,\rho} = \wp^\nu P^\rho$. For given $\rho = \rho_\mu$, the quantum number ν takes two possible values, $\nu = \pm 1$. Therefore all multi–dimensional irreps of D_n are two–dimensional and are labelled by $E_{|\mu|}$.

Using (8-10) and (8-37a) we get

$$C_{2x} P^\rho = P^{\rho^*} C_{2x}. \tag{8-38}$$

From (8-33b), (8-37b) and (8-38) we obtain the $D_n \supset C_{2x}$ and $\bar{D}_n \supset \bar{C}_n$ projection operator,

$$\begin{cases} \mathcal{P}^{(E_{|\mu|})}_{\nu,\mu} = \wp^\nu P^\mu = \left[P^\mu + P^{-\mu} C_{2x}\right], \\ \mathcal{P}^{(E_{|\mu|})}_{-\nu,\mu} = \frac{1}{i}\wp^{-\nu} P^\mu = \frac{1}{i}\left[P^\mu - P^{-\mu} C_{2x}\right], \end{cases} \quad \nu = 1, \tag{8-39a}$$

with the range of $|\mu|$

$$|\mu| = 1, 2, \ldots \left[\tfrac{n-1}{2}\right]. \tag{8-39b}$$

The phase factor $\frac{1}{i}$ in (8-39a) is chosen so as to conform with the standard phase conventions of Bradley & Cracknell (1972).

The universality and compactness of the expression $\wp^\nu P^\rho$ for the projection operators of D_n are to be noted. It is valid for both s–v and d–v representations (see Sec. 8.12.3), and for one– or two–dimensional irreps of D_n with *any integer n*. Although both one– and two–dimensional irreps have the same form of projection operator, $\wp^\nu P^\rho$, there are essential differences between the two. For the former both the operators C_{nz} and C_{2x} have definite values $\rho(= \pm 1)$ and $\nu(= \pm 1)$ with ν serving as a part of the irrep label, while for the latter the operators $\bar{C}_{nz}$ (rather than C_{nz}) and C_{2x} have definite values $\rho(=$ complex) and $\nu(= \pm 1)$ with ν serving as the component index.

8.5.3. The $D_n \supset C_n$ generalized projection operators

According to (8-33a) the $D_n \supset C_n, \bar{D}_n \supset \bar{C}_{2x}$ generalized projection operators are

$$\mathcal{P}^{(E_{|\mu|})}_{\mu,\nu} = P^\mu \wp^\nu, \ \mu = \pm|\mu|, \ \nu = 1, \tag{8-40a}$$

where the intrinsic quantum number ν could take ± 1, and the reason that we take $\nu = 1$ is for fixing the phase for the representation matrix. It is easy to verify that the representation matrix of the operator C_{2x} in the basis (8-40a) is

$$D^{E_\mu}(C_{2x}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{8-40b}$$

8.5.4. The $D_n \supset C_n$ projection operators

The $D_n \supset C_n$ projection operator can be obtained from the product of the generalized projection operator in (8-40a) and its Hermitian conjugate,

$$\begin{aligned} \mathcal{P}^{(E_{|\mu|})}_{\mu,\bar{\mu}} &= \mathcal{P}^{(E_{|\mu|})}_{\mu,\nu} \mathcal{P}^{(E_{|\mu|})}_{\nu,\bar{\mu}} = P^\mu \wp^\nu P^{\bar{\mu}} \\ &= P^\mu \delta_{\mu,\bar{\mu}} + \nu P^\mu C_{2x} \delta_{\mu,-\bar{\mu}}, \end{aligned} \tag{8-41a}$$

where (8-37b) and (8-38) has been used. From (8-41a) we get the $D_n \supset C_n$ projection operators

$$\begin{cases} \mathcal{P}^{(E_{|\mu|})}_{\mu,\mu} = P^\mu, \\ \mathcal{P}^{(E_{|\mu|})}_{-\mu,\mu} = P^{-\mu} C_{2x}, \end{cases} \quad \mu = \pm|\mu|. \tag{8-41b}$$

It can be verified that the representations carried by the $D_n \supset C_n$ projection operators in (8-41b) is identical to those carried by the generalized projection operators in (8-40a). It is what one expects due to our consistent choice of the value of $\nu = 1$ for both cases.

It is interesting to note that a single quantum number μ is sufficient to label a basis vector of any two–dimensional irrep of D_n, which belongs to the first (second) component for $\mu > 0$ ($\mu < 0$) of the irrep $E_{|\mu|}$.

From (8-39a) and (8-41b) we obtain the relation between the $D_n \supset C_{2x}$ generalized projection operators and the $D_n \supset C_n$ projection operators:

$$\begin{pmatrix} \mathcal{P}^{(E_\mu)}_{1,\mu} \\ \mathcal{P}^{(E_\mu)}_{-1,\mu} \end{pmatrix} = \mathcal{B} \begin{pmatrix} \mathcal{P}^{(E_\mu)}_{\mu,\mu} \\ \mathcal{P}^{(E_\mu)}_{-\mu,\mu} \end{pmatrix}, \quad \mu > 0, \tag{8-42a}$$

$$\mathcal{B} = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}. \tag{8-42b}$$

8.5.5. The $D_n \supset C_{2x}$ projection operators

We can use (8-33d) to construct the $D_n \supset C_{2x}$ projection operators. However, the simplest way to get them is from the $D_n \supset C_n$ generalized projection operators shown in (8-40a) through the following similarity transformation:

$$\begin{pmatrix} \mathcal{P}^{(E_\mu)}_{1,1} \\ \mathcal{P}^{(E_\mu)}_{-1,1} \end{pmatrix} = \mathcal{B} \begin{pmatrix} \mathcal{P}^{(E_\mu)}_{\mu,1} \\ \mathcal{P}^{(E_\mu)}_{-\mu,1} \end{pmatrix}, \quad \mu > 0. \tag{8-43a}$$

From (8-40a), (8-42b), (8-43a) and $\mathcal{P}^{(E_\mu)}_{\nu,-\nu} = (\mathcal{P}^{(E_\mu)}_{-\nu,\nu})^\dagger$, we get

$$\begin{cases} \mathcal{P}^{(E_\mu)}_{\nu,\nu} = \wp^\nu \mathcal{A}^\nu = \mathcal{A}^\nu \wp^\nu, \\ \mathcal{P}^{(E_\mu)}_{-\nu,\nu} = \wp^{-\nu} \mathcal{B}^\nu = \mathcal{B}^\nu \wp^\nu, \end{cases} \tag{8-43b}$$

where

$$\mathcal{A}^\nu = \sum_{k=0}^{n-1} \cos(\varphi_k) C^k_{nz}, \ \varphi_k = \tfrac{2k\mu\pi}{n}, \tag{8-43c}$$

$$\mathcal{B}^\nu = \mathrm{sign}(\nu) \sum_{k=0}^{n-1} \sin(\varphi_k) C^k_{nz}\,. \tag{8-43d}$$

For example, letting $n = 3, \mu = 1$ we obtain the $D_3 \supset C_{2x}$ single–valued projection operators

$$\begin{aligned} \mathcal{P}^{(E)}_{\nu,\nu} &= \tfrac{1}{\sqrt{12}} \wp^\nu (2e - C_{3z} - C^2_{3z}), \\ \mathcal{P}^{(E)}_{-\nu,\nu} &= \tfrac{1}{2} \mathrm{sign}(\nu) \wp^{-\nu} (C_{3z} - C^2_{3z}). \end{aligned} \tag{8-44}$$

8.5.6. The characters and irreducible matrices of D_n

Now let us find the irreducible matrices. A distinguishing feature of the algebraic expressions of the projection operators in (8-37c), (8-41b) and (8-43b) is that they are only functions of the quantum number (ρ, ν), or $(|\mu|, \nu)$, instead of depending on the irreducible matrix elements of all operators; yet they contain all information about the irreducible matrices. Using (8-32a), (8-36b) and (8-37a), from the projection operators given in (8-37c) and (8-41b) we can write out the irreducible matrices in the $D_n \supset C_n$ basis:

$$D^{A_{\rho\nu}}(C^k_{nz}) = \rho^k, \qquad D^{A_{\rho\nu}}(C_{2k}) = \nu\rho^k,$$

$$D^{E_\mu}(C_{nz}^k) = \begin{pmatrix} \rho^k, & 0 \\ 0, & \rho^{*k} \end{pmatrix}, \quad D^{E_\mu}(C_{2k}) = \begin{pmatrix} 0, & \rho^k \\ \rho^{*k}, & 0 \end{pmatrix}, \tag{8-45a}$$

or in a more explicit form,

$$D^{E_\mu}(C_{nz}^k) = \begin{pmatrix} e^{-\varphi_k i}, & 0 \\ 0, & e^{\varphi_k i} \end{pmatrix}, \quad D^{E_\mu}(C_{2k}) = \begin{pmatrix} 0, & e^{-\varphi_k i} \\ e^{\varphi_k i}, & 0 \end{pmatrix}. \tag{8-45b}$$

The irreducible matrices in the $D_n \supset \mathcal{C}_{2x}$ basis, denoted as $\mathbf{D}^{E\mu}$, can be obtained from those for the $D_n \supset C_n$ basis by a similarity transformation:

$$\mathbf{D}^{E_\mu}(R_a) = \mathcal{B}^* D^{E_\mu}(R_a)\tilde{\mathcal{B}}, \tag{8-46a}$$

with the results

$$\mathbf{D}^{E_\mu}(C_{nz}^k) = \begin{pmatrix} \cos\varphi_k, & -\sin\varphi_k \\ \sin\varphi_k, & \cos\varphi_k \end{pmatrix}, \mathbf{D}^{E_\mu}(C_{2k}) = \begin{pmatrix} \cos\varphi_k, & \sin\varphi_k \\ \sin\varphi_k, & -\cos\varphi_k \end{pmatrix}. \tag{8-46b}$$

It is seen that they are all real for single-valued reps, in agreement with the convention in Bradley & Cracknell (1972), and $\mathbf{D}^{E_\mu}(C_{2k})$ are symmetric, which is one of the advantages of our phase convention.

We can also write down the irreducible matrices from the $D_n \supset \mathcal{C}_{2x}$ projection operators given in (8-43b), and found that they are the same as (8-46b).

From (8-46b) (and (8-147b) for double-valued irreps) we can easily get the numerical results for the irreducible matrices of all the crystallographic dihedral groups shown in Table 8.5-1 and Table 8.5-2.

From (8-45) we get the algebraic expression for the characters of D_n

$$\chi^{A_{\rho\nu}}(C_{nz}^k) = \rho^k, \qquad \chi^{A_{\rho\nu}}(C_{2k}) = \nu\rho^k, \tag{8-47a}$$

$$\chi^{E_\mu}(C_{nz}^k) = 2\cos(\tfrac{2k\mu\pi}{n}), \qquad \chi^{E_\mu}(C_{2k}) = 0. \tag{8-47b}$$

We can use Eq. (8-47) to reproduce the character tables in Tables 8.3-2 to 8.3-7.

8.5.7. The symmetry adapted functions

The $O_3 \supset G \supset G(s)$ irreducible basis $\phi_{\lambda\mu}^l$ is called the *symmetry adapted functions* (SAF's) , which can be expressed in terms of homogeneous polynomials of x, y, and z, or in terms of $r^l Y_{lm}$, or simply in terms of the Y_{lm}, since r is invariant. The SAF's have important applications in physics. As mentioned in Sec. 3.19, the $O_3 \supset G \supset G(s)$ irreducible basis $\phi_{\lambda\mu}^l$ is the approximate (without considering the mixing of different orbitals l) wave function of an atom in a crystal field with symmetry G. The SAF's of dihedral groups have been tabulated in Altmann & Herzig (1994). However, compact algebraic expressions for the SAF's of dihedral groups can be derived using the projection operators.

The $D_n \supset \mathcal{C}_{2x}$ projection operators in (8-43b) are more complicated than the generalized projection operators in (8-39a) and with the latter it is much easier to construct the SAF's. The advantages of writing the projection operators in the form (8-37c) and (8-39a) are that they do not contain explicitly any of the irreducible matrix elements and each contains only two terms. With these projection operators it is almost trivial to obtain the SAF's.

1. Homogeneous Polynomials of (x, y, z) as SAF's

For dihedral groups it is very convenient to use the cylindrical coordinates (z, ρ, ϕ) with $\rho = \sqrt{x^2 + y^2}$. Since $z^{2p}\rho^k$ are invariants of D_n, we only need to consider the SAF's in the form of $f(\phi)$ and $zf(\phi)$, which can be easily converted to homogeneous polynomials of (x, y, z) with the help of the Maple software. Since the factor $z^{2p}\rho^k$ is "trivial" which can be easily added,

Table 8.5-1. The two-dimensional s-v and d-v irreducible matrices of $D_4 \supset C_{2x}$, $C_{4v} \supset C_{2x}$, $D_{2d} \supset C_{2x}$, $D_2 \supset C_{2x}$ and $C_{2v} \supset C_{2x}$.
$D_2 = \{E, C_{2z}, C_{2x}, C_{2y}\}$; $C_{2v} = \{E, C_{2z}, \sigma_x, \sigma_y\}$.
The matrices of D_2 and C_{2v} can be read off by ignoring the rows labelled by E_1, $E_{3/2}$ and $E_{5/2}$, and columns not belonging to their elements.

D_4	E	C_{4z}^+	C_{2z}	C_{4z}^-	C_{20}	C_{21}	C_{22}	C_{23}
C_{4v}	E	C_{4z}^+	C_{2z}	C_{4z}^-	σ_0	σ_1	σ_2	σ_3
D_{2d}	E	S_{4z}^-	C_{2z}	S_{4z}^+	C_{20}	σ_0	C_{21}	σ_1
E_1	ϵ	ρ	$-\epsilon$	$-\rho$	λ	κ	$-\lambda$	$-\kappa$
$E_{1/2}$	ϵ	$\frac{1}{\sqrt{2}}(\epsilon+\rho)$	ρ	$\frac{1}{\sqrt{2}}(\epsilon-\rho)$	$i\lambda$	$\frac{i}{\sqrt{2}}(\lambda+\kappa)$	$i\kappa$	$\frac{i}{\sqrt{2}}(\kappa-\lambda)$
$E_{3/2}$	ϵ	$\frac{1}{\sqrt{2}}(\rho-\epsilon)$	$-\rho$	$\frac{-1}{\sqrt{2}}(\epsilon+\rho)$	$i\lambda$	$\frac{i}{\sqrt{2}}(\kappa-\lambda)$	$-i\kappa$	$\frac{i}{\sqrt{2}}(\lambda+\kappa)$

Table 8.5-2. The two-dimensional s-v and d-v irreducible matrices of $D_6 \supset C_{2x}$, $C_{6v} \supset C_{2x}$, $D_{3h} \supset C_{2x}$, $D_3 \supset C_{2x}$ and $C_{3v} \supset C_{2x}$.
$D_3 = \{E, C_{3z}^+, C_{3z}^-, C_{20}, C_{22}, C_{24}\}$ is a subset of D_6.
$C_{3v} = \{E, C_{2z}^+, C_{3z}^-, \sigma_{0,}\sigma_2, \sigma_4\}$ is a subset of C_{6v}.
The matrices of D_3 and C_{3v} can be read off by ignoring the rows labelled by E_2, $E_{3/2}$ and $E_{5/2}$, and columns not belonging to their elements.

D_6	E	C_{6z}^+	C_{3z}^+	C_{2z}	C_{20}	C_{21}	C_{22}	C_{23}	C_{24}	C_{25}
C_{6v}	E	C_{6z}^+	C_{3z}^+	C_{2z}	σ_0	σ_1	σ_2	σ_3	σ_4	σ_5
D_{3h}	E	S_{3z}^-	C_{3z}^+	σ_z	C_{20}	$\theta\sigma_2$	C_{21}	σ_0	C_{22}	σ_1
E_1	ϵ	$-\beta$	α	$-\epsilon$	λ	$-\mu$	ν	$-\lambda$	μ	$-\nu$
E_2	ϵ	α	β	ϵ	λ	ν	μ	λ	ν	μ
$E_{1/2}$	ϵ	$\hat{\nu}$	$-\beta$	ρ	$i\lambda$	$-i\hat{\alpha}$	$-i\mu$	$i\kappa$	$i\nu$	$-i\hat{\beta}$
$E_{3/2}$	ϵ	ρ	$-\epsilon$	$-\rho$	$i\lambda$	$i\kappa$	$-i\lambda$	$-i\kappa$	$i\lambda$	$i\kappa$
$E_{5/2}$	ϵ	$\hat{\mu}$	$-\alpha$	ρ	$i\lambda$	$-i\hat{\beta}$	$i\mu$	$i\kappa$	$i\mu$	$-i\hat{\alpha}$

Table 8.5-3 Matrices appearing in Table 8.5-1 and Table 8.5-2.
The matrices $\hat{\alpha}$,$\hat{\beta}$,$\hat{\mu}$,$\hat{\nu}$ are obtained from α,β,μ,ν, respectively, by interchanging their two columns.

ϵ	κ	α	β
$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$
λ	ρ	μ	ν
$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$

we call a SAF *reduced* if it dose not involve $z^{2p}\rho^k$. Furthermore, we call a reduced SAF *fully reduced* if it consists of the simplest polynomials of (x,y,z) for given order of the polynomials. The fully reduced SAF's can be regarded as the building blocks for constructing SAF's of higher orders of polynomials of (x,y,z).

We first note that acting on the $SO(2)$ basis $e^{im\phi}$, the projection operator P^μ in (8-37a) will only pick out the state with $m = \mu \pmod n$,

$$P^\mu e^{im\phi} = \sum_{k=0}^{n-1} (\rho_\mu^* \rho_m)^k e^{im\phi} = n\dot{\delta}_{\mu m} e^{im\phi}, \tag{8-48a}$$

where (3-221b) has been used; $\dot{\delta}_{\mu m} = 1$ when $m = \mu \pmod n$ and zero otherwise. Applying the projection operators in (8-37c) and (8-39a) to $\exp(im\phi)$ and $z\exp(im\phi)$, and ignoring the irrelevant normalization factors we can obtain the $D_n \supset C_{2x}$ reduced SAF's as shown in Table 8.5-4. To obtain the SAF's in polynomials of (x,y,z), we only need to use the relations about the triangle functions.

For example, let us consider the group D_4. From the A_1 line in Table 8.5-4 we get the SAF ψ^{A_1} as $\rho^4\cos 4\phi = \rho^4(1 - 8\cos^2\phi\sin^2\phi) = \rho^4 - 8x^2y^2$. Deleting the "trivial" term $\rho^4 = (x^2+y^2)^2$, we are left with the fully reduced SAF, $\psi^{A_1} = x^2y^2$. Similarly, from the E_μ line we get $\psi_1^E = \rho^3\cos 3\phi = \rho^3(4\cos^3\phi - 3\cos\phi) = 4x^3 - 3\rho^2 x$. Deleting the second term which has already been known, we get the fully reduced SAF $\psi_1^E = x^3$. Notice that $\cos 3\phi$ can be written in another form, $\psi_1^E = \rho^3\cos 3\phi = \rho^3(\cos^3\phi - 3\cos\phi\sin^2\phi) = x^3 - 3xy^2$. Deleting the first term which has been found moments ago, and changing the sign in the second term, we get the fully reduced SAF $\psi_1^E = xy^2$. Analogously the second component of the irrep E can be obtained using $-\sin 3\phi = 4\sin^3\phi - 3\sin\phi = \sin^3\phi - 3\sin\phi\cos^2\phi$.

In this way we obtained the fully reduced SAF's of D_4 for up to fourth polynomials of (x,y,z) shown in Table 8.5-5.

2. Linear Combinations of $|jm\rangle$ as SAF's

Before finding the SAF's we first give the SAF's for the cyclic group C_n. Applying the projection operator P^μ in (8-37a) to $|jm\rangle$, or $|lm\rangle = Y_{lm}$ and use the following result,

$$P^\mu|jm\rangle = n\dot{\delta}_{\mu m}|jm\rangle, \tag{8-48b}$$

we get

$$\text{SAF's of } C_n : \varphi^{(\mu)} = |jm\rangle, \quad m = \mu \pmod n. \tag{8-48c}$$

Similarly applying the projection operator in (8-37c) to $|jm\rangle$ and using (8-48b) and

$$C_{2x}|jm\rangle = (-)^{-j}|j-m\rangle, \tag{8-48d}$$

we obtain the one-dimensional SAF's of D_n:

a. One-dimensional irreps

$$\psi^{A_{\rho\nu}} = |jm\rangle + (-)^j\nu|j-m\rangle, \quad \nu = \pm 1 \tag{8-49a}$$

$$\rho = \begin{cases} 1, \\ -1, \end{cases} \quad m = \begin{cases} 0 \pmod n, & n = \text{even or odd}, \\ \frac{n}{2} \pmod n, & n = \text{even}. \end{cases} \tag{8-49b}$$

b. Two-dimensional irreps

(1) In the $D_n \supset C_n$ basis

Applying the projection operators in (8-41b) to $|jm\rangle$ we obtain

Table 8.5-4. $D_n \supset C_{2x}$ s–v reduced SAF's in cylindrical coordinates. The SAF's are obtained by multiplying the reduced SAF's by $z^{2p}\rho^k$.

irrep	$m \pmod n$	reduced SAF	reduced SAF
A_1	0	$\cos m\phi$	$z\sin m\phi$
A_2	0	$\sin m\phi$	$z\cos m\phi$
B_1	$n/2$	$\cos m\phi$	$z\sin m\phi$
B_2	$n/2$	$\sin m\phi$	$z\cos m\phi$
E_μ $\mu = 1, 2, \ldots[\frac{n-1}{2}]$	μ	$(\cos m\phi, \sin m\phi)$	$z(\sin m\phi, -\cos m\phi)$

Table 8.5-5. $D_4 \supset C_{2x}$ s–v fully reduced SAF's for up to fourth order polynomials in (x, y, z). The fully reduced SAF is the SAF consisting of the simplest polynomials of (x, y, z).

irrep	m(mod 4)	reduced SAF	f. reduced SAF	reduced SAF	f. reduced SAF
A_1	0	$\cos 4\phi$	x^2y^2	$z\sin 4\phi$	$(x^3y - y^3x)z$
A_2	0	$\sin 4\phi$	$x^3y - y^3x$	$z\cos 4\phi$	x^2y^2z
B_1	2	$\cos 2\phi$	$x^2 - y^2$	$z\sin 2\phi$	xyz
B_2	2	$\sin 2\phi$	xy	$z\cos 2\phi$	$(x^2 - y^2)z$
E	1	$(\cos\phi, \sin\phi)$	(x, y)	$z(\sin\phi, -\cos\phi)$	$(y, -x)z$
	-3	$(\cos 3\phi, -\sin 3\phi)$	(x^3, y^3)	$z(\sin 3\phi, \cos 3\phi)$	$(-y^3, x^3)z$
			(xy^2, x^2y),		$(-x^2y, xy^2)z$

$$\begin{cases} \psi_\mu^{E_\mu} = |jm\rangle, \\ \psi_{-\mu}^{E_\mu} = (-)^j|j - m\rangle, \end{cases} \quad \mu > 0,\ m = \mu \pmod n, \tag{8-49c}$$

where the range of μ is given in (8-39b), while $m = \mu, \mu - n, \mu + n, \cdots$ under the restriction $|m| \le j$.

(2) In the $D_n \supset C_{2x}$ basis.

Similarly, from (8-39a) we have

$$\begin{cases} \psi_1^{E_\mu} = \left[|jm\rangle + (-)^j|j - m\rangle\right], \\ \psi_{-1}^{E_\mu} = \frac{1}{i}\left[|jm\rangle - (-)^j|j - m\rangle\right], \end{cases} \quad m = \mu \pmod n. \tag{8-49d}$$

In Eq. (8-49) the quantum number m is subject to the condition $|m| \le j$ and serves as the multiplicity label for the subduction $SO_3 \downarrow D_n$.

The SAF's are valid for both single–particle and many–particle cases. Notice that the SAF's of D_n for the latter case depend on the total angular momentum j but are independent of the parity, while for single–particle case where $j = l$, the SAF's do depend on the parity.

8.5.8. The group D_∞ (for both s–v and d–v reps)

The solutions for D_∞ can be obtained from those for D_n by letting $n \to \infty$, that is by letting

$$\phi_k = \tfrac{2k\pi}{n} \to \varphi,\ C_{nz}^k \to R_z(\varphi),\ C_{2k} \to C_2^{(\varphi/2)}, \tag{8-50a}$$

where $C_2^{(\varphi/2)}$ is obtained by rotating C_{2x} through an angle $\varphi/2$ about the z–axis.

The group C_∞ is a semi–direct product of $C_\infty (= SO(2))$ and C_{2x},

$$D_\infty = SO(2) \wedge C_{2x} = \{R_z(\varphi), C_2^{(\varphi)} : 0 \le \varphi < 2\pi\}. \tag{8-50b}$$

The group D_∞ has only two one–dimensional irreps $A_{\mu_0,\nu} = A_{0,\nu}$, $\nu = \pm 1$. In Mulliken notation those irreps are A_1 and A_2.

Characters and irreducible matrices

From equations (8-50a) and (8-47) we get the characters of D_∞,

$$\begin{aligned} &\text{One–dimensional: } \chi^{A_{0\nu}}(R_z(\varphi)) = 1, && \chi^{A_{0\nu}}(C_2^{(\varphi)}) = \nu, \\ &\text{Two–dimensional: } \chi^{E_\mu}(R_z(\varphi)) = 2\cos(\mu\varphi), && \chi^{E_\mu}(C_2^{(\varphi)}) = 0, \end{aligned} \tag{8-50c}$$

where $\nu = \pm 1$ and $\mu = \frac{1}{2}, 1, \frac{3}{2}, \cdots$.

From (8-50a) and (8-45) we obtain the irreducible matrices in the $D_\infty \supset C_\infty$ basis,

$$D^{E_\mu}(\varphi) = \begin{pmatrix} e^{-\mu\varphi i} & 0 \\ 0 & e^{\mu\varphi i} \end{pmatrix}, \; D^{E_\mu}(C_2^{(\varphi/2)}) = (-1)^\xi \begin{pmatrix} 0, & e^{-\mu\varphi i} \\ e^{\mu\varphi i}, & 0 \end{pmatrix}. \tag{8-50d}$$

where $\xi = 0(\frac{1}{2})$ for s–v (d–v) reps.

The $D_\infty \supset C_\infty$ symmetry adapted functions

From Eq. (8-49) we obtain

$$\begin{aligned} &\psi^{A_{0\nu}} = [1 + (-)^j \nu]|j, 0\rangle, \\ &\psi_\mu^{E_\mu} = |j\mu\rangle, \; \psi_{-\mu}^{E_\mu} = (-)^{j+\xi}|j - \mu\rangle. \end{aligned} \tag{8-50e}$$

8.5.9. Improper dihedral groups C_{nv}, D_{nd} (even n) and D_{nh} (odd n)

The improper dihedral groups C_{nv}, D_{nh}, D_{nd} can be treated similarly (Chen, Fan, et al, 2000). It can be shown that the expression for the characters and irreducible matrices of D_n apply to the improper dihedral groups with the correspondence between the elements of D_n and those of the improper dihedral groups shown in Table 8.5-1 and Table 8.5-2.

A significant difference between the SAF's of proper dihedral groups and improper dihedral groups is that the former is independent of the parity , while the latter does. Therefore we need to specify the parity of the state $|jm\rangle$ explicitly by writing $|\ell jm\rangle$ with parity $(-1)^\ell = \pm 1$. Using the correspondence of the operators indicated in the table headings of Table 8.5-3 and Table 8.5-4, it can be shown (Chen, Fan, et al, 2000) that the SAF's of improper dihedral groups can be easily found from those of D_n with $|jm\rangle$ replaced by $|\ell jm\rangle$ and using the following simple rules.

The groups C_{nv}: The SAF's of C_{nv} with even parity are identical to the SAF's of D_n,

$$\psi_\sigma^\Gamma(\ell = \text{even})|_{C_{nv}} = \psi_\sigma^\Gamma|_{D_n}, \quad \Gamma = A_{\rho\nu}, E_\mu, \; \sigma = \mu, \nu, \tag{8-51a}$$

while the $C_{nv} \supset C_n$ SAF's of odd parities can be obtained from those of even parities by

$$\psi^{A_{\rho,\nu}}(\ell = \text{odd}) = \psi^{A_{\rho,-\nu}}(\ell = \text{even}), \tag{8-51b}$$

$$\psi_\mu^{E_{|\mu|}}(\ell = \text{odd}) = \text{sign}(\mu)\psi_\mu^{E_{|\mu|}}(\ell = \text{even}), \tag{8-51b}$$

where $\text{sign}(\mu) = \pm 1$ for $\mu = \pm|\mu|$.

The groups D_{nd} and D_{nh}: The SAF's of D_{nd} and D_{nh} with even parity are identical to the SAF's of D_{2n},

$$\psi_\sigma^\Gamma(\ell = \text{even})|_{D_{nd}} = \psi_\sigma^\Gamma|_{D_{2n}}, \quad \Gamma = A_{\rho\nu}, E_\mu, \; \sigma = \mu, \nu, \tag{8-52a}$$

while the SAF's of D_{nd} and D_{nh} with odd parities can be obtained from those of even parities by

$$\psi^{A_{\rho,\nu}}(\ell = \text{odd}) = \psi^{A_{-\rho,\nu}}(\ell = \text{even}), \tag{8-52b}$$

$$\psi_\sigma^{E_{|\mu|}}(\ell = \text{odd}) = \psi_\sigma^{E_{n-|\mu|}}(\ell = \text{even})|_{m\to -m},\ \sigma = \mu, \nu. \tag{8-52c}$$

With the irreducible matrices shown in Table 8.5-3 to Table 8.5-5 for the improper dihedral groups, the CG coefficients of an improper dihedral group are identical to those of the proper dihedral groups to which it is isomorphic. The algebraic expressions for the CG coefficients of all dihedral groups are given in Chen, Fan et al (2000).

Ex. 8.9. Use the criterion for irreducibility given in Sec. 2.11 to prove that the representation E_μ given in (8-45) is irreducible.

Ex. 8.10. From (8-47) and (8-46) construct the character table and irreducible matrices of the group D_6, and compare them with Table 8.3-6 and Table 8.5-2.

Ex. 8.11. In analogy with Table 8.5-5, construct the $D_6 \supset C_{2x}$ s–v fully reduced SAF's.

Ex. 8.12. Find the SAF's of $C_{nv} \supset C_{2x}$ and check (8-51). *Hints*: 1. The projection operators of C_{nv} are given in (8-37) and (8-39) with C_{2x} replaced by σ_x. 2. Using $\sigma_x|\ell jm\rangle = (-1)^{\ell-j}|\ell j - m\rangle$.

Ex. 8.13. Find the SAF's of D_{nd} and D_{nh} using (8-52).

8.6. Numerical Solutions for $T \supset D_2$ and $O \supset D_4 \supset D_2$

In many textbooks, the explicit form of irreducible bases of the cubic groups in terms of the lowest possible polynomials of x, y and z are given without explicitly specifying to which subgroup chains they are symmetry adapted. By looking at which operators they are eigenfunctions of, we can find the corresponding operator set $C(s)$, and then the subgroup chain $G(s)$. For the group T a commonly used basis is the $T \supset D_2$ basis, while for the group $O(T_d)$, two kinds of irreducible bases are often used, the real basis $O_h \supset D_4 \supset D_2 (T_d \supset D_{2d} \supset D_2)$ and the complex basis, $O_h \supset C_4$ $(T_d \supset S_4)$. These bases are listed in Table 8.6-1 to Table 8.6-3.

We could use the method of Sec. 3.13 to get the irreducible matrices of the cubic groups by decomposing their regular reps. However, with simple polynomials of x, y and z as the basis functions listed in Table 8.6, we can easily derive the irreducible matrices of the cubic groups without decomposing the regular rep.

For example, according to the transformation of the coordinates $(x, y, z)[(yz, xz, xy)]$ under the operation of the group O, we can obtain the irrep $F_1[F_2]$ of the group O. From Fig. 8.2-5, we get

$$xyz \xrightarrow{C_{4z}^+} \bar{y}xz, \quad xyz \xrightarrow{C_{2\zeta}} \bar{z}\bar{y}\bar{x}, \tag{8-53}$$

where $\bar{x} \equiv -x$. From the above, we have

$$C_{4z}^+ \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -y \\ x \\ z \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} .$$

Therefore the representation matrix for C_{4z} in the irrep F_1 is [compare this result with (2-59)]

$$D^{F_1}(C_{4z}^+) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} .$$

Table 8.6-1. The basis and basis functions of T.

$$Y_{20} = \sqrt{\tfrac{5}{16\pi}}(2z^2 - x^2 - y^2),\ Y_{22}^c = \sqrt{\tfrac{5}{16\pi}}\sqrt{3}(x^2 - y^2).$$

	C	$C(s)$	$T \supset D_2$
	$4C_3$	(C_{2x}, C_{2y})	$T \supset D_2$
A_0	4		$x^2+y^2+z^2$
A_1	$4\exp(-2\pi i/3)$		$\frac{1}{\sqrt{2}}[Y_{20} + iY_{22}^c]$
A_{-1}	$4\exp(2\pi i/3)$		$\frac{1}{\sqrt{2}}[Y_{20} - iY_{22}^c]$
F	0	$(+-,-+,--)$	$(x,y,z);(yz,xz,xy)$

Table 8.6-2. Bases and basis functions of T_d.

$$f^{A_2} = x^4(y^2 - z^2) + y^4(z^2 - x^2) + z^4(x^2 - y^2),$$
$$R_x = x(y^2 - z^2), \text{cyclic in } x, y, z.$$

	C		$C(s)$	
	$6S_4$	$T_d \supset D_{2d} \supset D_2$ basis	S_{4z}^-	$T_d \supset S_4$ basis
A_1	6	$x^2+y^2+z^2$	1	$x^2+y^2+z^2$
A_2	-6	f^{A_2}	-1	f^{A_2}
E	0	(Y_{20}, Y_{22}^c)	$(1,-1)$	(Y_{20}, Y_{22}^c)
F_1	2	(R_x, R_y, R_z)	$(-i,i,1)$	$-\sqrt{\frac{1}{2}}(R_x + iR_y), \sqrt{\frac{1}{2}}(R_x - iR_y), R_z$
F_2	-2	$(x,y,z);(yz,xz,xy)$	$(-i,i,-1)$	$-\sqrt{\frac{1}{2}}(x+iy), \sqrt{\frac{1}{2}}(x-iy), z$

Table 8.6-3. Bases and basis functions of $O, O_h = O \times C_i$

	C			$C(s)$	
	$6C_4$,	I	$O_h \supset D_4 \supset D_2$ basis	C_{4z}^+	$O_h \supset C_4$ basis
A_{1g}	6,	1	$x^2+y^2+z^2$	1	$x^2+y^2+z^2$
A_{2g}	-6,	1	f^{A_2}	-1	f^{A_2}
E_g	0,	1	(Y_{20}, Y_{22}^c)	$(1,-1)$	(Y_{20}, Y_{22}^c)
F_{1g}	2,	1	R_x, R_y, R_z	$(-i,i,1)$	$-\sqrt{\frac{1}{2}}(R_x + iR_y), \sqrt{\frac{1}{2}}(R_x - iR_y), R_z$
F_{2g}	-2,	1	(yz, xz, xy)	$(-i,i,-1)$	$-\sqrt{\frac{1}{2}}(yz + ixz), \sqrt{\frac{1}{2}}(yz - ixz), xy$
A_{1u}	6,	-1	$xyzf^{A_2}$	1	$xyzf^{A_1}$
A_{2u}	-6,	-1	xyz	-1	xyz
E_u	0,	-1	$xyz(Y_{20}, Y_{22}^c)$	$(1,-1)$	$xyz(Y_{20}, Y_{22}^c)$
F_{1u}	2,	-1	x, y, z	$(-i,i,1)$	$-\sqrt{\frac{1}{2}}(x+iy), \sqrt{\frac{1}{2}}(x-iy), z$
F_{2u}	-2,	-1	$x(y^2-z^2), y(z^2-x^2), z(x^2-y^2)$	$(-i,i,-1)$	

From (8-53) we can also get

$$C_{4z}^{+}\begin{pmatrix} yz \\ xz \\ xy \end{pmatrix} = \begin{pmatrix} xz \\ -yz \\ -yx \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\begin{pmatrix} yz \\ xz \\ xy \end{pmatrix} .$$

Thus

$$D^{F_i}(C_{4z}^{+}) = (-1)^{i+1}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad i = 1, 2 . \tag{8-54a}$$

Analogously, we can obtain

$$D^{F_i}(C_{4x}^{+}) = (-1)^{i+1}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} , \quad D^{F_i}(C_{4y}^{+}) = (-1)^{i+1}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} ,$$

$$D^{F_i}(C_{2e}) = (-1)^{i}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} , \qquad D^{E}(C_{2e}) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} . \tag{8-54b}$$

where $i = 1, 2$, the basis for the irrep $F_1[F_2]$ of O is $(x, y, z)[(yz, xz, xy)]$. The matrix C_{4x}^{-} is related to that of C_{4x}^{+} by $D^{F_i}(C_{4x}^{-}) = \tilde{D}^{F_i}(C_{4x}^{+})$, similarly for C_{4y}^{-} and C_{4z}^{-}.

The $O \supset D_4 \supset D_2$ irreducible matrices of all elements are tabulated in McWeeny (1963). However for finding the CG coefficients by the EFM, we only need the irreducible matrices of the elements contained in the CSCO–II. As will be seen, Eq. (8-54) is all we need.

The irreps of the group T_d are also given by Eq. (8-54) with the following replacements:

$$C_{2e} \to \sigma_{de} , \qquad C_{4z}^{+} \to S_{4z}^{-} .$$

However one should notice that $(x, y, z)[(yz, xz, xy)]$ carries the irrep $F_2[F_1]$ of the group T_d.

The irreducible matrices of the group O_h can be written down immediately from those of the group O by using (8-29) with χ replaced by D.

The $G \supset G(s)$ irreducible basis $\psi_{\mu}^{(\lambda)}$ of a point group G satisfies the eigenvalue equations

$$\begin{pmatrix} C \\ C(s) \end{pmatrix}\psi_{\mu}^{(\lambda)} = \begin{pmatrix} \lambda \\ \mu \end{pmatrix}\psi_{\mu}^{(\lambda)} . \tag{8-55a}$$

According to Eq. (3-262), for irreps with dimension greater than one, it suffices to find the solution to (8-55a) for a single component μ of the irrep λ. Choosing appropriate operators $\mathcal{O}$ and using the irreducible matrices $D(\mathcal{O})$ given above, we can obtain the other components $\psi_{\mu'}^{(\lambda)}$ of the same irrep λ from the following equation

$$\psi_{\mu'}^{(\lambda)} = \frac{1}{D_{\mu'\mu}^{(\lambda)}(\mathcal{O})}\left[\mathcal{O} - D_{\mu\mu}^{(\lambda)}(\mathcal{O})\right]\psi_{\mu}^{(\lambda)} . \tag{8-55b}$$

The CSCO–II for the group chain $O \supset C_4$ is (C, C_{4z}^{+}), while the CSCO–II for $O \supset D_4 \supset D_2$ is (C, C_{D_4}, C_{D_2}), which consists of five operators and is not convenient to use. From Table 8.6-3 it is seen that the two components of the irrep E and the third component of the irrep F_i in the $O \supset D_4 \supset D_2$ classification are the same as in the $O \supset C_4$ scheme. Therefore for finding the $O \supset D_4 \supset D_2$ irreducible basis we can solve Eq. (8-55a) with $C(s) = C_{4z}^{+}$ to obtain the first component of the irrep E, and the third component of the irrep F_i, and further use Eq. (8-56) below, to find the second component of the irrep E and the first and second components of the irrep F_i (for the ordering of the components, see Tables 8.6-3).

The same applies to the $T_d \supset D_{2d} \supset D_2$ group chain by replacing O, D_4, C_{4z}^+ with T_d, D_{2d}, S_{4z}^-, respectively.

Using Eq. (8-54), (8-55b) can be put into the following explicit form tailored for the group chains $T_d \supset D_{2d} \supset D_2$ and $O \supset D_4 \supset D_2$,

$$\begin{array}{lll} & \text{The group } T_d & \text{The group } O \\ T_d \supset S_{4z}: & \psi_2^E = \sqrt{\frac{1}{3}}[2\sigma_{de}+1]\psi_1^E\,, & O \supset C_{4z}: \ \psi_2^E = \sqrt{\frac{1}{3}}[2C_{2e}+1]\psi_1^E\,, \\ T_d \supset D_{2d} \supset D_2: & \psi_1^{F_i} = (-1)^i\sigma_{de}\psi_3^{F_i}\,, & O \supset D_4 \supset D_2: \ \psi_1^{F_i} = (-1)^i C_{2e}\psi_3^{F_i}, i=1,2\,, \\ & \psi_2^{F_i} = (-1)^i\sigma_{df}\psi_3^{F_i}\,. & \psi_2^{F_i} = (-1)^i C_{2f}\psi_3^{F_i}\,. \end{array} \tag{8-56}$$

8.7. Algebraic Solutions for Cubic Groups

8.7.1. Double-Coset factored projection operators and their application

In physics one often uses the canonical group chain $G \supset C_n$ for a point group. For example the group chains $T \supset C_3, O \supset C_4, I \supset C_5$. The projection operators for such cases can be greatly simplified by using double-coset factorization (Zhang & Li 1986). In (1-26) we introduced the *double-coset decomposition.* By replacing H with C_n we have

$$G = C_n(e+\beta_2+\cdots+\beta_p)+C_n(\beta_{p+1}+\cdots+\beta_q)C_n. \tag{8-57a}$$

For example we have

$$T = C_3 + C_3C_{2z}C_3, \quad C_3 = \{e, C_{31}^+, C_{31}^-\}, \tag{8-57b}$$

$$O = C_4(e+C_{2y})+C_4C_{2b}C_4, \quad C_4 = \{e, C_{4z}^+, C_{2z}^+, C_{4z}^-\}. \tag{8-57c}$$

Suppose that $f(a)$ is a function on the group G and $d(\beta_j)$ is the frequency that an element R_a occurs in the double coset $C_n\beta_jC_n$. Using

$$\sum_{a\in G} f(a) = \sum_{i,k=1}^{n}\sum_{j=1}^{q}\frac{1}{d(\beta_j)}f(C_{nz}^i\beta_jC_{nz}^k),$$

and

$$D_{\rho,\bar{\rho}}^{(\lambda)}(C_{nz}^i\beta_jC_{nz}^k) = \rho^i D_{\rho,\bar{\rho}}^{(\lambda)}(\beta_j)\bar{\rho}^k\,, \tag{8-58}$$

the $G \supset C_n$ projection operator can be expressed as

$$\begin{aligned} \mathcal{P}_\rho^{(\lambda)\bar{\rho}} &= \sqrt{\tfrac{h_\lambda}{|G|}}\sum_{a=1}^{|G|} D_{\rho,\bar{\rho}}^{(\lambda)}(R_a)^* R_a \\ &= \sqrt{\tfrac{h_\lambda}{|G|}}\sum_{j=1}^{p}\sum_{i=1}^{n}(\rho^*)^i D_{\rho,\bar{\rho}}^{(\lambda)}(\beta_j)^* C_{nz}^i\beta_j \\ &\quad + \sqrt{\tfrac{h_\lambda}{|G|}}\sum_{j=p+1}^{q}\sum_{i,k=1}^{n}(\rho^*)^i D_{\rho,\bar{\rho}}^{(\lambda)}(\beta_j)^*(\bar{\rho}^*)^k C_{nz}^i\beta_jC_{nz}^k \\ &= \sqrt{\tfrac{h_\lambda}{|G|}}\left[\sum_{j=1}^{p} D_{\rho,\bar{\rho}}^{(\lambda)}(\beta_j)^* P^\rho\beta_j + \sum_{j=p+1}^{q} D_{\rho,\bar{\rho}}^{(\lambda)}(\beta_j)^* P^\rho\beta_jP^{\bar{\rho}}\right] \end{aligned} \tag{8-59}$$

where P^ρ is the unnormalized projection operator of C_n (8-37a).

Equation (8-59) is the *double-coset factored projection operator*, which depends only on the irreducible matrices of the q double-coset representatives instead of all the $|G|$ elements of the group, and thus is a great simplification over its original form. By applying it to $|jm\rangle$ and using [Cf. (8-48b)]

$$P^{\mu}|j\bar{m}\rangle = n\dot{\delta}_{\mu,\bar{m}}|j\bar{m}\rangle,\ \beta_i|j\bar{m}\rangle = \sum_m \mathcal{D}^j_{m\bar{m}}(\beta_i)|jm\rangle, \tag{8-60a}$$

where $\mathcal{D}^j_{m\bar{m}}$ is the D function of rotation group, we obtain the $G \supset C_n$ unnormalized SAF (Zhang & Li 1986):

$$\psi^{(\lambda)\bar{m}}_{\mu} = \sum_m{}' \left[\sum_{i=1}^{p} D^{(\lambda)}_{\mu,\bar{\mu}}(\beta_i)^* \mathcal{D}^j_{mm}(\beta_i)\dot{\delta}_{m\bar{m}} + n \sum_{i=p+1}^{q} D^{(\lambda)}_{\mu,\bar{\mu}}(\beta_i)^* \mathcal{D}^j_{mm}(\beta_i) \right] |jm\rangle, \quad \bar{m} \doteq \bar{\mu}, \tag{8-60b}$$

where $\bar{m} \doteq \bar{\mu}$ means $\bar{m} = \bar{\mu} \pmod n$, while $\sum'$ means that the summation is subjected to the condition $m \doteq \mu$. With given $G \supset C_n$ irreducible matrices $D^{(\lambda)}_{\mu,\bar{\mu}}(\beta_i)^*$ for the coset generators, from (8-60b) one can calculate the $G \supset C_n$ SAF's.

8.7.2. Algebraic expressions for the $T \supset C_3$ projection operator

Although the double-coset factored projection operator greatly simplifies the projection operator method, it still contains the irreducible matrices of all coset generators. Our task in this section is to introduce a method for finding algebraic expressions of the projection operators for non-dihedral groups G which are merely functions of the quantum numbers $\lambda, \mu, \bar{\mu}$ of the group chain $G \supset G(s)$,

$$\mathcal{P}^{(\lambda)\bar{\mu}}_{\mu} = f(\lambda, \mu, \bar{\mu}), \tag{8-60c}$$

without involving explicitly the irreducible matrices of any elements. Once the algebraic expression (8-60c) is found, the irreducible matrices, characters, SAF's and CG coefficients all can be obtained easily. The algebraic expressions of the $G \supset C_n$ projection operators have been found for all point groups in Chen & Fan (1998, 1999) and Fan, Chen & Draayer (1999). In the following we only deal with the $T \supset C_3$ s-v case.

The starting point of finding algebraic solutions for a group is to construct its group table. The group table of T can be read off from the group table of O in Table 10.21-1 and is given in Table 8.7-1.

Table 8.7-1. The group table of $T^{\dagger}$ (For s-v reps, $\tilde{R} = R$.)

1	E	1	2	3	4	5	6	7	8	9	10	11	12
2	C_{2x}	2	$\tilde{1}$	4	$\tilde{3}$	$\tilde{8}$	7	$\tilde{6}$	5	10	$\tilde{9}$	12	$\widetilde{11}$
3	C_{2y}	3	$\tilde{4}$	$\tilde{1}$	2	$\tilde{6}$	5	8	$\tilde{7}$	11	$\widetilde{12}$	$\tilde{9}$	10
4	C_{2z}	4	3	$\tilde{2}$	$\tilde{1}$	$\tilde{7}$	$\tilde{8}$	5	6	12	11	$\widetilde{10}$	$\tilde{9}$
5	C^+_{31}	5	$\tilde{6}$	$\tilde{7}$	$\tilde{8}$	$\tilde{9}$	12	10	11	1	3	4	2
6	C^+_{32}	6	5	8	$\tilde{7}$	11	$\widetilde{10}$	12	9	$\tilde{3}$	1	$\tilde{2}$	4
7	C^+_{33}	7	$\tilde{8}$	5	6	12	9	$\widetilde{11}$	10	$\tilde{4}$	2	1	$\tilde{3}$
8	C^+_{34}	8	7	$\tilde{6}$	5	10	11	9	$\widetilde{12}$	$\tilde{2}$	$\tilde{4}$	3	1
9	C^-_{31}	9	12	10	11	1	$\tilde{2}$	$\tilde{3}$	$\tilde{4}$	$\tilde{5}$	7	8	6
10	C^-_{32}	10	$\widetilde{11}$	$\tilde{9}$	12	2	1	$\tilde{4}$	3	8	$\tilde{6}$	5	7
11	C^-_{33}	11	10	$\widetilde{12}$	$\tilde{9}$	3	4	1	$\tilde{2}$	6	8	$\tilde{7}$	5
12	C^-_{34}	12	$\tilde{9}$	11	$\widetilde{10}$	4	$\tilde{3}$	2	1	7	5	6	$\tilde{8}$

The $T \supset C_3$ normalized projection operator is

$$\mathcal{P}_{\rho}^{(\lambda)\bar{\rho}} = \sqrt{\frac{h_\lambda}{12}} \sum_{a=1}^{12} D_{\rho\bar{\rho}}^{(\lambda)}(R_a)^* R_a, \tag{8-61a}$$

This obeys the simultaneous eigenvalue equations,

$$(C, C_{31}^+, \bar{C}_{31}^+)\mathcal{P}_{\rho}^{(\nu)\bar{\rho}} = (\lambda, \rho, \bar{\rho})\mathcal{P}_{\rho}^{(\lambda)\bar{\rho}}. \tag{8-61b}$$

The eigenvalue of C_{31}^+ is denoted by $\rho \equiv \rho_\mu$, where

$$\rho = \rho_\mu = \exp(-\tfrac{2\pi\mu i}{3}),\ \mu = 0, \pm 1. \tag{8-61c}$$

Our task is to seek simultaneous eigenvectors of $(C, C_{31}^+, \bar{C}_{31}^+)$. The simultaneous eigenvectors of $(C_{31}^+, \bar{C}_{31}^+)$ are easily constructed as

$$\begin{aligned} &\varphi_{\bar{\rho}\rho}^1 = \delta_{\rho\bar{\rho}}\varphi_\rho^1, \qquad \varphi_\rho^1 = \tfrac{1}{\sqrt{3}}P^\rho, \\ &\varphi_{\rho\bar{\rho}}^2 = \tfrac{1}{3}P^\rho C_{2z} P^{\bar{\rho}}, \end{aligned} \tag{8-62a}$$

where P^ρ is an eigenvector of C_{31}^+, that is the projection operator of C_3,

$$P^\mu \equiv P^{\rho_\mu} = e + \rho C_{31}^- + \rho^* C_{31}^+ = \mathbf{1} + \rho\mathbf{9} + \rho^*\mathbf{5}, \tag{8-62b}$$

where here and in the following we use bold face integers to denote the group element listed in Table 8.7-1. For example **5** represents the element $R_5 = C_{31}^+$.

The two basis vectors $\varphi_{\rho\bar{\rho}}^1$, $\varphi_{\rho\bar{\rho}}^2$ form what is called the *double-induced representation* , a representation of T induced from the irrep of $(\rho, \bar{\rho})$ of the group $C_3 \times \bar{C}_3$. Notice that there are only $12 = 1 \times 3 + 1 \times 3^2$ linearly independent basis vectors in (8-62a).

Using the group table, the two common eigenvectors of C_{31}^+ and $\bar{C}_{31}^+$ can be written explicitly,

$$\begin{aligned} &\varphi_\rho^1 = \tfrac{1}{\sqrt{3}}\big[\mathbf{1} + \rho\mathbf{9} + \rho^*\mathbf{5}\big], \\ &\varphi_{\rho\bar{\rho}}^2 = \tfrac{1}{3}\big[(\mathbf{4} + \rho\mathbf{11} + \rho^*\mathbf{8}) + \bar{\rho}(\mathbf{12} + \rho\mathbf{6} + \rho^*\mathbf{2}) + \bar{\rho}^*(\mathbf{7} + \rho\mathbf{3} + \rho^*\mathbf{10})\big]. \end{aligned} \tag{8-62c}$$

For later convenience, one element in each of the basis vectors of the double–induced rep is chosen as its representative. Although any element in a basis vector can be chosen as its representative, the simplest choice here is to choose the element **1** and **4** as the representatives of φ^1 and φ^2.

The task of finding the eigenvectors of the CSCO–III in the 12–dimensional group space of T is reduced to finding the eigenvector of the CSCO in the two–dimensional double–induced rep space $L_{\rho\bar{\rho}} = \{\varphi_{\rho\bar{\rho}}^i : i = 1, 2\}$.

We need to linearly combine $\varphi_{\rho\bar{\rho}}^1$ and $\varphi_{\rho\bar{\rho}}^2$ into eigenvectors of C. So the next step is to find the representation matrix M of the operator C in the double–induced representation. A key point for finding the matrix elements M_{ji} in $C\varphi_{\rho\bar{\rho}}^i = \sum_j M_{ji}\varphi_{\rho\bar{\rho}}^j$, is that we only need to find the coefficients in front of the representatives of $\varphi_{\rho\bar{\rho}}^1$ and $\varphi_{\rho\bar{\rho}}^2$, that is in front of **1** and **4**. This can be accomplished by highlighting the elements **1** and **4** in rows 5–8 (which correspond to the elements $C_{31}^+ - C_{34}^+$) of the group table of T, then collecting the highlighted numbers in each column. This gives the table

R_i	**9**	**10**	**11**	**12**
CR_i	**1** + **4**	**1**+ **4**	**1**+**4**	**1** +**4**

The table shows, for example, that $CR_9 = R_1 + R_4 + \cdots$. The terms involving elements other than R_1 and R_4 are ignored. Using the above table and (8-62c) we have

$$\begin{aligned} C\varphi^1_\rho &= \tfrac{1}{\sqrt{3}}\rho(\mathbf{1}+\mathbf{4}) = \rho\varphi^1_\rho + \sqrt{3}\rho\varphi^2_{\rho\rho} \\ C\varphi^2_{\rho\bar\rho} &= \tfrac{1}{3}[\rho + \bar\rho + (\bar\rho\rho)^*](\mathbf{1}+\mathbf{4}) \\ &= \sqrt{3}\rho\varphi^1_\rho\delta_{\rho\bar\rho} + (\rho + \bar\rho + \rho^*\bar\rho^*)\varphi^2_{\rho\bar\rho}, \end{aligned} \tag{8-63a}$$

From (8-63a) we obtain the rep matrix M of C,

$$M = \begin{pmatrix} \rho\delta_{\rho\bar\rho} & \sqrt{3}\rho\delta_{\rho\bar\rho} \\ \sqrt{3}\rho\delta_{\rho\bar\rho} & \rho + \bar\rho + (\rho\bar\rho)^* \end{pmatrix}. \tag{8-63b}$$

Since $\rho \equiv \rho_\mu = \exp(-\frac{2\pi\mu i}{3})$, there is a one–to–one correspondence between ρ_μ and μ. In the following we switch to the μ notation.

The diagonalization of the matrix M in (8-63b) is carried out separately for two cases:

Case (i) $\rho \neq \bar\rho$

When $\bar\rho \neq \rho$, or $\bar\mu \neq \mu$, M shrinks into one–dimensional and there is only one non–vanishing vector, $\varphi^2_{\mu\bar\mu}$, which is necessarily an eigenvector of the operator C with the eigenvalue $\lambda = M_{22} = \rho_\mu + \rho_{\bar\mu} + (\rho_\mu\rho_{\bar\mu})^*$,

$$\lambda = 0, \quad \text{for } (\mu,\bar\mu) \text{ or } (\bar\mu,\mu) = (1,-1),(0,1),(0,-1). \tag{8-63c}$$

Consulting Table 8.6-1 we find that the eigenvalues $\lambda = 0$ correspond to the irrep F. Hence we have the basis vectors

$$\mathcal{P}^{(\lambda=0)\bar\mu}_\mu = \mathcal{P}^{(F)\bar\mu}_\mu = \varphi^2_{\mu\bar\mu}, \quad \mu \neq \bar\mu = 0, \pm 1. \tag{8-64a}$$

Case (ii) $\bar\rho = \rho$

For $\rho = \bar\rho$, the matrix M is simplified as

$$M = \rho_\mu \begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & 3 \end{pmatrix}. \tag{8-63d}$$

The eigenvector is

$$\mathcal{P}^{(\lambda)\mu}_\mu = N_{\lambda\mu}\left[\varphi^1_\mu - \tfrac{1}{\sqrt{3}}(1 - \lambda\rho_{-\mu})\varphi^2_{\mu\mu}\right]. \tag{8-64b}$$

For each μ, the matrix M in (8-63d) has two eigenvalues, which are easily found as

$$\lambda = (0,\ 4\rho_\mu), \quad \mu = 0, \pm 1. \tag{8-64c}$$

Equation (8-64a,b) give the algebraic expressions of the projection operators as a function of $\lambda, \mu, \bar\mu$. These expressions are very elegant if the quantum number λ is used as irrep label. Unfortunately, most are not familiar with this new labelling scheme and therefore it is more convenient to change back to the Mulliken notation. According to Table 8.6-1, the eigenvalue $\lambda = 4\rho_\mu$ corresponds to the one–dimensional irreps A_μ, $\mu = 0, \pm 1$. Substituting the eigenvalues (8-64c) into (8-64b), we can get the projection operators in a more explicit but less compact form,

$$\begin{cases} \mathcal{P}^{(A_\mu)} = \frac{1}{2}(\varphi^1_\mu + \sqrt{3}\varphi^2_{\mu\mu}), \\ \mathcal{P}^{(F)\mu}_\mu = \frac{1}{2}(\sqrt{3}\varphi^1_\mu - \varphi^2_{\mu\mu}), \end{cases} \quad \mu = 0, \pm 1. \tag{8-64d}$$

From (8-62a) , (8-64a) and (8-64d) we get all the $T \supset C_3$ projection operators

$$\begin{cases} \mathcal{P}^{(A_\mu)} = \frac{1}{\sqrt{12}}\left[P^\mu + P^\mu C_{2z} P^\mu\right], \\ \mathcal{P}^{(F)\mu}_{\mu} = \frac{1}{2}\left[P^\mu - \frac{1}{3}P^\mu C_{2z} P^\mu\right], \quad \mu = 1, 0, -1. \\ \mathcal{P}^{(F)\bar{\mu}}_{\mu} = \frac{1}{3}P^\mu C_{2z} P^{\bar{\mu}}, \bar{\mu} \neq \mu, \end{cases} \tag{8-65}$$

8.7.3. The $T \supset C_3$ irreducible matrices

The algebraic expressions for the projection operators in (8-65) are only functions of the quantum numbers $\lambda, \mu, \bar{\mu}$ and are thus very concise. Nonetheless they contain essentially all the information about the irreducible matrix elements. To construct SAF's a knowledge of the projection operators is sufficient. However if one needs to find the CG coefficients, a knowledge of the irreducible matrices of the coset generators is also required, which can be found in the following way.

The operator C_{31}^+ is diagonal and its representation matrix is known, $D^F_{\mu\mu'}(C_{31}^+) = \delta_{\mu\mu'}\rho_\mu$. The representation matrix of the coset generator C_{2z} is obtained in the following way. Comparing (8-65) with (8-59) we see that the coefficients of $P^\mu C_{2z} P^{\bar{\mu}}$ in (8-65) are equal to $\sqrt{\frac{h_\lambda}{|G|}} D^\lambda_{\mu\bar{\mu}}(C_{2z})^*$. Consequently, from (8-65), we immediately get the $T \supset C_3$ matrix elements of C_{2z}, $D^F_{\mu\mu'}(C_{2z}) = \frac{2}{3} - \delta_{\mu\mu'}$, or in matrix form

$$D^F(C_{31}^+) = \begin{pmatrix} \rho_1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \rho_{-1} \end{pmatrix}, \quad D^F(C_{2z}) = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}. \tag{8-66a}$$

If one needs the irreducible matrices of other elements, they can be obtained by the following simple formulas,

$$D^{(\lambda)}_{\mu\bar{\mu}}(C_{31}^j C_{2z} C_{31}^k) = \rho_\mu^j D^{(\lambda)}_{\mu\bar{\mu}}(C_{2z})\rho_{\bar{\mu}}^k = \epsilon^{\mu j + \bar{\mu} k} D^{(\lambda)}_{\mu\bar{\mu}}(C_{2z}), \tag{8-66b}$$

where $C_{31}^j \equiv (C_{31}^+)^j$. Using the group table of T we can obtain the pair of index (j,k) for each element of $T^\dagger$, as shown below.

(j,k)	(00)	(01)	(02)	(10)	(11)	(12)	(20)	(21)	(22)
$C_{31}^j C_{2z} C_{31}^k$	C_{2z}	C_{33}^+	C_{34}^-	C_{34}^+	C_{32}^-	C_{2x}	C_{33}^-	C_{2y}	C_{32}^+

Eq. (8-66b) shows that the irreducible matrix elements of all elements in the same double-coset differ from that of the coset generator by only a phase factor $\epsilon^{\mu j + \bar{\mu} k}$. Eq. (8-66) are the algebraic expressions for the irreducible matrices of T.

8.7.4. The algebraic expressions for $T \supset C_3$ SAF's

In obtaining the SAF's, the normalization of the projection operators is unimportant and for each irrep we only need one set of the projection operators. We collect these chosen unnormalized projection operators below, and call them the "generalized" projection operators. Taking $\bar{\mu} = 0$ for the irrep F from (8-65) we obtain the $T \supset C_3$ "generalized" projection operators

$$\begin{cases} \mathbf{P}^{A_\mu} = P^\mu + P^\mu C_{2z} P^\mu, \\ \mathbf{P}^F_\mu = 3P^\mu \delta_{\mu 0} - (-1)^\mu P^\mu C_{2z} P^{\bar{\mu}=0}, \end{cases} \quad \mu = 1, 0, -1. \tag{8-67}$$

The projection operator method with the projection operator in its original form (8-61a) is quite tedious, but it becomes very efficient with the algebraic form in (8-67).

Up to now the coordinate system has not been specified explicitly. For obtaining the SAF's we need to introduce the coordinate system. The usual coordinate system for the group T is

shown in Fig. 8.2-3, with the Euler angles of C_{2z} as $C_{2z} = R(0,0,\pi)$. For obtaining the $T \supset C_3$ SAF's, we choose the coordinate system $x'y'z'$ as shown in Fig. 8.7-1, with z' as the axis of C_{31}^{+}. The coordinate system $x'y'z'$ is obtained from the system xyz in Fig. 8.2-3 by a rotation $R(\omega)$,

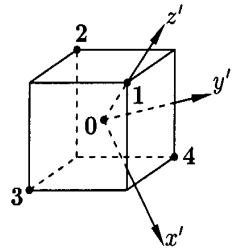


Fig. 8.7-1 The coordinate system $x'y'z'$ for $T \supset C_3$

$$xyz \overset{R(\omega)}{\to} x'y'z', \; R(\omega) \equiv R\big(\tfrac{\pi}{4}, \cos^{-1}\tfrac{1}{\sqrt{3}}, 0\big). \tag{8-68a}$$

Notice that $\cos^{-1}\frac{1}{\sqrt{3}}$ is the angle between the z axis and the axis of C_{31}^{+} in Fig. 8.2-3. The Euler angles $(\alpha'\beta'\gamma')$ of C_{2z} in the system $x'y'z'$ are given by

$$C_{2z} = R(\alpha'\beta'\gamma') = R(\omega)^{-1}R(0,0,\pi)R(\omega) = R\big(\pi, \; \cos^{-1}(-\tfrac{1}{3}), \; 0\big). \tag{8-68b}$$

The SAF's can be obtained by applying the projection operator to a trial state $|l\bar{m}\rangle (= Y_{lm})$, or $|l\bar{m}\rangle \pm |l - \bar{m}\rangle$, according to convenience. We choose

$$\psi^{(A_\mu)\bar{m}} = \mathbf{P}^{A_\mu}|j\bar{m}\rangle, \quad \psi_\mu^{(\Gamma)\bar{m}} = \mathbf{P}_\mu^{\Gamma}\big[|j\bar{m}\rangle + \mathrm{sign}(\bar{m})|j - \bar{m}\rangle\big], \Gamma = A_0, F. \tag{8-68c}$$

Using

$$P^{\mu}|j\bar{m}\rangle = 3\dot{\delta}_{\mu,\bar{m}}|j\bar{m}\rangle, \; C_{2z}|j\bar{m}\rangle = \sum_m e^{-im\pi} d^j_{m\bar{m}}(\beta_0)|jm\rangle, \; \beta_0 = \cos^{-1}(-\tfrac{1}{3}),$$

and (8-68c) we immediately obtain the $T \supset C_3$ SAF's:

1. One-dimensional irreps

$$\psi^{(A_0)\bar{m}} = Y_{l\bar{m}} \pm Y_{l-\bar{m}} + 3\sum_{m \doteq 0} (-1)^m \left[d^l_{m\bar{m}}(\beta_0) \pm d^l_{m-\bar{m}}(\beta_0)\right] Y_{lm}, \quad \bar{m} \doteq 0, \tag{8-69a}$$

$$\psi^{(A_\mu)\bar{m}} = Y_{l\bar{m}} + 3\sum_{m \doteq \mu} (-1)^m d^l_{m\bar{m}}(\beta_0) Y_{lm}, \quad \bar{m} \doteq \mu, \; \mu = \pm 1, \tag{8-69b}$$

where $m \doteq \mu$ stands for $m = \mu, \mu + 3, \mu - 3, \cdots$, and the normalization factor is suppressed for simplicity.

2. Three-dimensional irreps

$$\psi_\mu^{(F)\bar{m}} = (Y_{l\bar{m}} \pm Y_{l-\bar{m}})\delta_{\mu,0} - (-1)^\mu \sum_{m \doteq \mu} (-)^m \left[d^l_{m\bar{m}}(\beta_0) \pm d^l_{m-\bar{m}}(\beta_0)\right] Y_{lm},$$

$$\bar{m} \doteq 0, \; \mu = 0, \pm 1. \tag{8-69c}$$

Notice that the index $\bar{m}$ in (8-69) serves as the multiplicity label. When an irrep λ occurs only once in D^l, $\bar{m}$ may take any permissible value, say the lowest possible value, i. e. zero for the irrep A_0 or F, and ± 1 and for the irrep $A_{\pm 1}$. The results with different $\bar{m}$ differ at most by

an overall phase. When an irrep λ occurs τ times, we need to let $\bar{m}$ taking τ different values, $0, 3, -3, 6, -6, \cdots$ for A_0 or F, $1, -2, 4, -5, \cdots$ for A_1 and $-1, 2, -4, 5, \cdots$ for A_{-1}. According to our experience the τ sets of SAF's $\psi_\mu^{(\lambda)\bar{m}}$ are always linearly independent, though not orthogonal in $\bar{m}$. In practical calculation as a check we evaluate the determinant of the $\tau \times \tau$ overlap matrix

$$\det \left| \langle \psi_\mu^{(\lambda)\bar{m}} | \psi_\mu^{(\lambda)\bar{m}'} \rangle \right|,$$

for any given value of μ. If it is nonzero, than the τ sets of SAF's $\psi_\mu^{(\lambda)\bar{m}}$ are linearly independent.

With the algebraic expressions (8-69), it is easy to find the exact numerical expression of the SAF's $\psi_\mu^{(\Gamma)\bar{m}}$ for any l with the help of some software, say the Maple software. The multiplicity $\tau = \tau_\lambda^l$ for the occurrence of the irrep λ of T in the subduced rep $l \downarrow \lambda$ is calculated first by using (3-249b) or (8-71b) and used as a control parameter for the calculation. No orthogonalizing procedure is included to maintain and emphasize the simplicity of the algebraic expression of the SAF's. The $T \supset C_3$ SAF's for j =1–3, and a part for $j = 6, 8$ are listed in Table 8.7-2.

Table 8.7-2. The $T \supset C_3$ SAF's.

The superscript is the multiplicity label.

For l =6 and 8 only the SAF's with multiplicity are listed.

$\bar{m} = 0$

$|F\text{-}1\rangle = -|1\text{-}1\rangle$

$|F0\rangle = |10\rangle$

$|F1\rangle = |11\rangle$

$\bar{m} = -1$

$|A_{-1}\rangle = \frac{\sqrt{2\cdot 3}}{3}|2\text{-}1\rangle - \frac{\sqrt{3}}{3}|22\rangle$

$\bar{m} = 1$

$|A_1\rangle = \frac{\sqrt{3}}{3}|2\text{-}2\rangle + \frac{\sqrt{2\cdot 3}}{3}|21\rangle$

$\bar{m} = 0$

$|F\text{-}1\rangle = \frac{\sqrt{3}}{3}|2\text{-}1\rangle + \frac{\sqrt{2\cdot 3}}{3}|22\rangle$

$|F0\rangle = |20\rangle$

$|F1\rangle = \frac{\sqrt{2\cdot 3}}{3}|2\text{-}2\rangle - \frac{\sqrt{3}}{3}|21\rangle$

$\bar{m} = 0$

$|A_0\rangle = -\frac{\sqrt{2}}{3}|3\text{-}3\rangle + \frac{\sqrt{5}}{3}|30\rangle + \frac{\sqrt{2}}{3}|33\rangle$

$\bar{m} = 0$

$|F\text{-}1\rangle^1 = \frac{\sqrt{2\cdot 3}}{6}|3\text{-}1\rangle - \frac{\sqrt{2\cdot 3\cdot 5}}{6}|32\rangle$

$|F0\rangle^1 = \frac{\sqrt{2\cdot 5}}{6}|3\text{-}3\rangle + \frac{2}{3}|30\rangle - \frac{\sqrt{2\cdot 5}}{6}|33\rangle$

$|F1\rangle^1 = -\frac{\sqrt{2\cdot 3\cdot 5}}{6}|3\text{-}2\rangle - \frac{\sqrt{2\cdot 3}}{6}|31\rangle$

$\bar{m} = 3$

$|F\text{-}1\rangle^2 = -\frac{2\sqrt{3\cdot 5\cdot 7}}{21}|3\text{-}1\rangle + \frac{\sqrt{3\cdot 7}}{21}|32\rangle$

$|F0\rangle^2 = \frac{2\sqrt{7}}{21}|3\text{-}3\rangle - \frac{\sqrt{2\cdot 5\cdot 7}}{21}|30\rangle + \frac{\sqrt{7}}{3}|33\rangle$

$|F1\rangle^2 = \frac{4\sqrt{3\cdot 7}}{21}|3\text{-}2\rangle - \frac{\sqrt{3\cdot 5\cdot 7}}{21}|31\rangle$

$\bar{m} = 0$

$|A_0\rangle^1 = \frac{\sqrt{2\cdot 3\cdot 7\cdot 11}}{54}|6\text{-}6\rangle - \frac{\sqrt{3\cdot 5\cdot 7}}{27}|6\text{-}3\rangle + \frac{4\sqrt{2}}{9}|60\rangle + \frac{\sqrt{3\cdot 5\cdot 7}}{27}|63\rangle + \frac{\sqrt{2\cdot 3\cdot 7\cdot 11}}{54}|66\rangle$

$\bar{m} = 3$

$|A_0\rangle^2 = \frac{\sqrt{2\cdot 3\cdot 5}}{18}|6\text{-}6\rangle + \frac{\sqrt{3\cdot 11}}{9}|6\text{-}3\rangle + \frac{\sqrt{3\cdot 11}}{9}|63\rangle - \frac{\sqrt{2\cdot 3\cdot 5}}{18}|66\rangle$

$\bar{m} = -2$

$|A_1\rangle^1 = \frac{\sqrt{2\cdot 3\cdot 7\cdot 11\cdot 13}}{324}|8\text{-}8\rangle + \frac{\sqrt{3\cdot 5\cdot 11\cdot 13}}{81}|8\text{-}5\rangle + \frac{16\sqrt{3}}{81}|8\text{-}2\rangle - \frac{\sqrt{3\cdot 5\cdot 7}}{162}|81\rangle + \frac{11\sqrt{2\cdot 3\cdot 5\cdot 11}}{324}|84\rangle - \frac{\sqrt{3\cdot 7\cdot 11\cdot 13}}{162}|87\rangle$

$\bar{m} = 1$

$|A_1\rangle^2 = \frac{16\sqrt{3\cdot 5\cdot 11\cdot 13}}{81\sqrt{487}}|8\text{-}8\rangle - \frac{8\sqrt{2\cdot 3\cdot 7\cdot 11\cdot 13}}{81\sqrt{487}}|8\text{-}5\rangle - \frac{4\sqrt{2\cdot 3\cdot 5\cdot 7}}{81\sqrt{487}}|8\text{-}2\rangle + \frac{487\sqrt{2\cdot 3}}{81\sqrt{487}}|81\rangle + \frac{37\sqrt{3\cdot 7\cdot 11}}{81\sqrt{487}}|84\rangle + \frac{11\sqrt{2\cdot 3\cdot 5\cdot 11\cdot 13}}{81\sqrt{487}}|87\rangle$

$\bar{m} = -1$

$|A_{-1}\rangle^1 = \frac{11\sqrt{2\cdot 3\cdot 5\cdot 11\cdot 13}}{81\sqrt{487}}|8\text{-}7\rangle - \frac{37\sqrt{3\cdot 7\cdot 11}}{81\sqrt{487}}|8\text{-}4\rangle + \frac{487\sqrt{2\cdot 3}}{81\sqrt{487}}|8\text{-}1\rangle + \frac{4\sqrt{2\cdot 3\cdot 5\cdot 7}}{81\sqrt{487}}|82\rangle - \frac{8\sqrt{2\cdot 3\cdot 7\cdot 11\cdot 13}}{81\sqrt{487}}|85\rangle - \frac{16\sqrt{3\cdot 5\cdot 11\cdot 13}}{81\sqrt{487}}|88\rangle$

$\bar{m} = 2$

$|A_{-1}\rangle^2 = \frac{\sqrt{3\cdot 7\cdot 11\cdot 13}}{162}|8\text{-}7\rangle + \frac{11\sqrt{2\cdot 3\cdot 5\cdot 11}}{324}|8\text{-}4\rangle + \frac{\sqrt{3\cdot 5\cdot 7}}{162}|8\text{-}1\rangle + \frac{16\sqrt{3}}{81}|82\rangle - \frac{\sqrt{3\cdot 5\cdot 11\cdot 13}}{81}|85\rangle + \frac{\sqrt{2\cdot 3\cdot 7\cdot 11\cdot 13}}{324}|88\rangle$

8.7.5. SAF's for the group chain $O \supset T \supset C_3$

The algebraic solutions for the group chain $O \supset T \supset C_3$ have been found in Chen & Fan (1999) by using the right-induced technique, and the main results are summarized below. The

group O is a semi–direct product of T and a cyclic group $\mathcal{C}_2$ of order 2, $O = T \wedge \mathcal{C}_2$. The group O can be decomposed into right cosets

$$O = T(e + C_{2b}) \ .$$

Suppose that the algebraic expressions for the $T \supset C_3$ projection operators $\mathcal{P}_{\mu}^{(\lambda)\bar{\mu}}$ have been found in (8-65). By linearly combine the vectors $\mathcal{P}_{\mu}^{(\lambda)\bar{\mu}}$ and $\mathcal{P}_{\mu}^{(\lambda)\bar{\mu}} C_{2b}$ into eigenvectors of the CSCO of O, we can obtain the algebraic expression for the $O \supset T \supset C_3$ projection operators. Applying the projection operator to $|j\bar{m}\rangle$ we get the $O \supset T \supset C_3$ SAF's. The following extremely simple results have been found between the $O \supset T \supset C_3$ SAF's and the $T \supset C_3$ SAF's.

1. One–dimensional irreps

The SAF's $\psi^{(A_0)\bar{m}}|_{T \supset C_3}$ of the group T is the SAF's of the irreps A_σ of O with $\sigma = 1, 2$ determined by l and $\bar{m}$,

$$\begin{aligned} &\psi^{(A_\sigma)\bar{m}} = \psi^{(A_0)\bar{m}}|_{T \supset C_3}, \ \bar{m} = 0 \ (\mathrm{mod}\ 3), \\ &(-1)^\sigma = \mathrm{sign}(\bar{m})(-1)^{l+\bar{m}+1}. \end{aligned} \tag{8-70a}$$

2. Two–dimensional irrep

The SAF's of the irreps $A_{\pm 1}$ of T constitute the two components of the irrep E of the group O,

$$\begin{cases} \psi_{A_1}^{(E)\bar{m}} = \psi^{(A_1)\bar{m}}|_{T \supset C_3}, \\ \psi_{A_{-1}}^{(E)\bar{m}} = (-1)^{l-\bar{m}} \psi^{(A_{-1})-\bar{m}}|_{T \supset C_3}, \end{cases} \quad \bar{m} = 1 \ (\mathrm{mod}\ 3). \tag{8-70b}$$

3. Three–dimensional irreps

The SAF's $\psi^{(F)\bar{m}}|_{T \supset C_3}$ of the group T are the SAF's of the irrep F_σ of the group O with $\sigma = 1, 2$ determined by l and $\bar{m}$,

$$\begin{aligned} &\psi_{\mu}^{(F_\sigma)\bar{m}} = \psi_{\mu}^{(F)\bar{m}}|_{T \supset C_3}, \ \bar{m} = 0 \ (\mathrm{mod}\ 3), \\ &(-1)^\sigma = \mathrm{sign}(\bar{m})(-1)^{l+\bar{m}}. \end{aligned} \tag{8-70c}$$

The irreducible matrices of O in the group chain $O \supset T \supset C_3$ can be constructed from those of the coset generators. Therefore we only give the irreducible matrices of the double–coset generator C_{2z} of the group T (with respect to the subgroup C_3) and the right–coset generator C_{2b} of O (with respect to its subgroup T). The irreducible matrices $\mathcal{D}$ of the group O for the element C_{2z} is obtainable from those D of the group T by

$$\mathcal{D}^{\Gamma_\sigma}(C_{2z}) = D^{\Gamma}(C_{2z}), \ \Gamma = A, F; \ \mathcal{D}^{E}(C_{2z}) = D^{A_1}(C_{2z}) \oplus D^{A_{-1}}(C_{2z}), \tag{8-70d}$$

The irreducible matrices of C_{2b} are

$$\begin{aligned} &\mathcal{D}^{(A_\sigma)}(C_{2b}) = (-1)^{\sigma+1}, \\ &\mathcal{D}^{(E)}(C_{2b}) = \delta_{\mu-\bar{\mu}}, \ \mu, \bar{\mu} = \pm 1, \\ &\mathcal{D}^{(F_\sigma)}(C_{2b}) = (-1)^\sigma \delta_{\mu-\bar{\mu}}, \ \mu, \bar{\mu} = 0, \pm 1. \end{aligned} \tag{8-70e}$$

Algebraic solutions for point groups can greatly simplify the problem in solving the Schrödinger equations in molecular physics (Chen, Iachello & Ping 1996, Ping & Chen 1997).

From Sec. 5 and Sec. 7 it is seen that in our approach we start from finding the algebraic expressions of the projection operator $\mathcal{P}_{\mu}^{(\lambda)\bar{\mu}}$. Once we got it, the irreducible matrices and characters follow immediately. While in the standard approach, one starts from finding the primitive characters, and then the irreducible matrices, and using them to construct the projection operators, i. e., just in the reverse order.

The differences between the conventional induction method (Mackay 1968, Bradley & Cracknell 1972) are discussed in Chen & Fan (1998a).

8.7.6. The splitting of atomic levels in the $O_3 \supset G \supset G(s)$ basis

The symmetry of an atom placed in a crystal field with the point group symmetry G is lowered from O_3 to G, and its energy levels, originally characterized by l, will be split. According to (3-337d), the number of the sublevels is given by the subduction of the irrep $D^{(l)}$ of O_3 with respect to G,

$$D^{(l)} \downarrow G = \sum_{\lambda} \oplus \tau_\lambda D^{(\lambda)}(G) \,, \tag{8-71a}$$

where τ_λ is determined by (3-249b), that is,

$$\tau_\lambda = \sum_i \frac{g_i}{g} (\chi_i^\lambda)^* \chi_i^{l\downarrow G} \,. \tag{8-71b}$$

According to (6-64) and the fact that under the inversion $I, Y_{lm} \to (-)^l Y_{lm}$, we have

$$\chi^l(\varphi) = \frac{\sin(l+1/2)\varphi}{\sin(\varphi/2)} \times \begin{cases} 1 & \text{proper rotations} \,, \\ (-1)^l & \text{improper rotations} \,. \end{cases} \tag{8-72a}$$

Letting $\varphi = \frac{\pi}{2}$ in (8-72a) and noting that $\sigma_x = IC_{2x}$, we have

$$\chi^l(C_2) = (-1)^l \,, \qquad \chi^l(\sigma) = 1 \,. \tag{8-72b}$$

Setting φ to be some specific values compatible with the group elements of G, we can find from (8-72) the characters $\chi_i^{l\downarrow G}$ for the subduced rep of G.

Example 1: The splitting of atomic levels in the $\mathcal{C}_{4v}$ crystal field. The character $\chi^{l\downarrow\mathcal{C}_{4v}}$ for the subduced rep of $\mathcal{C}_{4v}$ is listed in Table 8.7-3. From Table 8.7-3, and the simple character of $\mathcal{C}_{4v}$ in Table 8.3-4, we can calculate the multiplicities τ_λ as listed in Table 8.7-4, which is called a compatibility table.

Table 8.7-3. The subduced character $\chi^{l\downarrow\mathcal{C}_{4v}}$.

l	e	C_{2z}	$2C_4^z$	2σ	$2\sigma'$
0	1	1	1	1	1
1	3	−1	1	1	1
2	5	1	−1	1	1
3	7	−1	−1	1	1
4	9	1	1	1	1

Table 8.7-4. Compatibility table for reps of O_3 and the point group $\mathcal{C}_{4v}$.

0	A_1
1	$A_1 + E$
2	$A_1 + B_1 + B_2 + E$
3	$A_1 + B_1 + B_2 + 2E$
4	$2A_1 + A_2 + B_1 + B_2 + 2E$

Ex. 8.14. Show that the $T \supset C_3$ SAF's have the symmetries:

$$\begin{cases} \left\langle \psi^{(A_0)\bar{m}} \middle| lm \right\rangle = (-1)^{m+\bar{m}} \text{sign}(\bar{m}) \left\langle \psi^{(A_0)\bar{m}} \middle| l-m \right\rangle, \\ \left\langle \psi^{(A_\mu)\bar{m}} \middle| lm \right\rangle = (-1)^{m+\bar{m}} \left\langle \psi^{(A_{-\mu})-\bar{m}} \middle| l-m \right\rangle, \ \mu = \pm 1, \\ \left\langle \psi_\mu^{(F)\bar{m}} \middle| lm \right\rangle = (-1)^{m+\bar{m}} \text{sign}(\bar{m}) \left\langle \psi_{-\mu}^{(F)\bar{m}} \middle| l-m \right\rangle, \ \mu = 0, \pm 1. \end{cases}$$

Check these symmetries in Table 8.7-2.

Ex. 8.15. Using (8-66) construct all the irreducible matrices for the irrep F of T.

Ex. 8.16. From the third component xy for the irrep F_1 of the group T_d, use (8-56) to find the first and second components.

Ex. 8.17. Find the compatibility table for the group $\mathcal{C}_{6v}$, for the O_3 irreps $l = 0, 1, 2, 3, 4, 5$ (the characters of $\mathcal{C}_{6v}$ are given in Table 8.3-6).

Ex. 8.18. Show that for $\mathcal{C}_{4v}$ and $\mathcal{C}_{6v}$ we have

$$D^{4n+k} = n \text{ reg} \oplus D^k, \quad (k = 0, 1, 2, 3), \qquad \text{for } \mathcal{C}_{4v},$$
$$D^{6n+k} = n \text{ reg} \oplus D^k, \quad (k = 0, 1, 2, 3, 4, 5), \quad \text{for } \mathcal{C}_{6v},$$

where "reg" stands for the regular representation of the group.

8.8. The CG Coefficients of Point Groups

8.8.1. The CG series of point groups

The CG series of the 32 point groups,

$$D^{(\lambda_1)} \times D^{(\lambda_2)} = \sum_{\lambda} \oplus (\lambda_1 \lambda_2 \lambda) D^{(\lambda)} , \tag{8-73}$$

were given by Koster (1963). As an example, Table 8.8-1 gives the CG series for the groups T_d and O. Due to the relation $(\lambda_1 \lambda_2 \lambda) = (\lambda_2 \lambda_1 \lambda)$, only the right upper triangle of the table is shown. For groups with real characters, the coefficients $(\lambda_1 \lambda_2 \lambda)$ also satisfy the relation (3-276).

Table 8.8-1. The CG series of the groups T_d and O.

	A_1	A_2	E	F_1	F_2
A_1	A_1	A_2	E	F_1	F_2
A_2		A_1	E	F_2	F_1
E			$A_1 + A_2 + E$	$F_1 + F_2$	$F_1 + F_2$
F_1				$A_1 + E + F_1 + F_2$	$A_2 + E + F_1 + F_2$
F_2					$A_1 + E + F_1 + F_2$

8.8.2. The CG coefficients of point groups

The CG coefficients of point groups are defined through the equation

$$\psi_{\mu}^{(\lambda)\tau}(x_1, x_2) = \sum_{\mu_1 \mu_2} C^{(\lambda)\tau,\mu}_{\lambda_1 \mu_1, \lambda_2 \mu_2} \varphi_{\mu_1}^{(\lambda_1)}(x_1) \varphi_{\mu_2}^{(\lambda_2)}(x_2) . \tag{8-74}$$

For the single–valued reps of the 32 crystal point groups, the multiplicity label τ is redundant. However, for the double–valued reps, the multiplicity can be larger than one (Koster 1963).

The CG coefficients of point groups can be calculated by the EFM [see (3-293)]. As an example, let us apply Eq. (3-293) to the Kronecker product $F_2 \times F_2$ of the group T_d in the group chain $T_d \supset D_{2d} \supset D_2$.

According to (3-294), the matrix elements of the CSCO–II, (C, S_{4z}^{-}), of T_d in the uncoupled rep can be expressed as

$$\langle i'j'|C|ij\rangle = \sum_a D_{i'i}^{(F_2)}(R_a) D_{j'j}^{(F_2)}(R_a) ,$$
$$\langle ii|C|jj\rangle = \sum_a [D_{ij}^{(F_2)}(R_a)]^2 , \tag{8-75a}$$

where the sum runs over $R_a = S_{4x}^+, \cdots, S_{4z}^-$;

$$\langle i'j'|S_{4z}^-|ij\rangle = D_{i'i}^{(F_2)}(S_{4z}^-)D_{j'j}^{(F_2)}(S_{4z}^-) \ . \tag{8-75b}$$

From (8-54) and (8-75) we obtain the representation matrices of C and S_{4z}^- in the uncoupled rep. Those matrices are block–diagonal with the submatrices

$$\mathbf{C} = \begin{array}{c} |11\rangle|22\rangle|33\rangle \\ \left(\begin{array}{ccc} 2 & 2 & 2 \\ 2 & 2 & 2 \\ 2 & 2 & 2 \end{array}\right) \end{array}, \quad \mathbf{S}_{4z}^- = \begin{array}{c} |11\rangle|22\rangle|33\rangle \\ \left(\begin{array}{ccc} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{array}\right) \end{array}, \tag{8-75c}$$

$$\mathbf{C} = \begin{array}{c} |12\rangle \quad |21\rangle \\ \left(\begin{array}{cc} 0 & -2 \\ -2 & 0 \end{array}\right) \end{array}, \quad \mathbf{S}_{4z}^- = \begin{array}{c} |12\rangle \quad |21\rangle \\ \left(\begin{array}{cc} 0 & -1 \\ -1 & 0 \end{array}\right) \end{array}. \tag{8-75d}$$

By diagonalizing the two matrices in (8-75c) simultaneously and consulting Table 8.6-2, we obtain the following three eigenvectors,

$$\begin{gathered} \Psi^{A_1} = \tfrac{1}{\sqrt{3}}(|11\rangle + |22\rangle + |33\rangle) \ , \\ \Psi_1^E = \tfrac{1}{\sqrt{6}}(-|11\rangle - |22\rangle + 2|33\rangle) \ , \quad \Psi_2^E = \tfrac{1}{\sqrt{2}}(|11\rangle - |22\rangle) \ . \end{gathered} \tag{8-76a}$$

The relative phase of the basis vectors of the irrep E cannot be fixed from the eigenequations. To ensure a consistent relative phase, we take a solution, say Ψ_1^E, from (8-76a), and then use (8-54) and (8-56) to find Ψ_2^E,which is,

$$\Psi_2^E = \tfrac{1}{\sqrt{3}}(2\sigma_{df} + 1)\Psi_1^E = \tfrac{1}{\sqrt{2}}(|11\rangle - |22\rangle) \ .$$

Similarly, a simultaneous diagonalization of the two matrices in (8-75d) gives

$$\Psi_3^{F_1} = \tfrac{1}{\sqrt{2}}(|12\rangle - |21\rangle) \ , \quad \Psi_3^{F_2} = \tfrac{1}{\sqrt{2}}(|12\rangle + |21\rangle) \ . \tag{8-76b}$$

By changing 1, 2, and 3 cyclically, we obtain the other two components. The CG coefficients of the group chains $O \supset D_4 \supset D_2$ and $T_d \supset D_{2d} \supset D_2$ are the same, and are listed in Table 8.8-2.

The CG coefficients of point groups are generally used to couple irreducible bases of two particles or two systems. However, they can also be used to couple two irreducible bases of the same particle. Letting $x_1 = x_2 = x$, in (8-74), if the resulting expression is not zero, then it is an unnormalized irreducible basis of the group G,

$$\psi_\mu^{(\lambda)}(x) = \sum_{\mu_1\mu_2} C_{\lambda_1\mu_1,\lambda_2\mu_2}^{\lambda,\mu} \varphi_{\mu_1}^{(\lambda_1)}(x)\varphi_{\mu_2}^{(\lambda_2)}(x) \ . \tag{8-77a}$$

For example, noting $|1\rangle = x, |2\rangle = y, |3\rangle = z$, we have from (8-76)

$$\begin{gathered} \psi^{A_1} = \tfrac{1}{\sqrt{3}}(x^2 + y^2 + z^2) \ , \quad \psi_1^E = \tfrac{1}{\sqrt{6}}(2z^2 - x^2 - y^2) \ , \quad \psi_2^E = \tfrac{1}{\sqrt{2}}(x^2 - y^2) \ , \\ \psi_3^{F_1} = \tfrac{1}{\sqrt{2}}(xy - yx) = 0 \ , \quad \psi_3^{F_2} = \sqrt{2}xy \ . \end{gathered} \tag{8-77b}$$

They are identical to the bases listed in Table 8.6-2, except for the normalization factors.

The CG coefficients of the point groups have been tabulated by Koster (1963), Butler (1981), Altmann & Herzig (1994). The CG coefficients of the crystallographic point groups symmetry adapted to any canonical group chains can be calculated by the code of Chen & Ping (1999)

Ex. 8.19. Calculate the CG coefficients for the products $E \times E$ and $F_1 \times F_2$ of the group O.

Ex. 8.20. Using the CG coefficients for the product $E \times F_2$ of T_d, show that $\psi^{l=3}_{(F_2)3} = Y_{30}$. Then use (8-56) to show that

$$\psi^{l=3}_{(F_2)1} = \tfrac{1}{4}[\sqrt{5}(Y_{33} + Y_{3-3}) - \sqrt{3}(Y_{31} + Y_{3-1})] ,$$
$$\psi^{l=3}_{(F_2)2} = -\tfrac{1}{4i}[\sqrt{5}(Y_{33} - Y_{3-3}) + \sqrt{3}(Y_{31} - Y_{3-1})] .$$

Ex. 8.21. Using Table 8.8-2 show that

$$\psi^{l}_{(F_1)3} = Y_{2l+1,0} , \quad \text{for the group } O ,$$
$$\psi^{l}_{(F_2)3} = Y_{2l+1,0} , \quad \text{for the group } T_d .$$

Table 8.8-2. The CG coefficients of the groups T_d and O. Here $-\frac{1}{2}$, for example, represents $-\sqrt{1/2}$.

$E \times E$	(11)	(12)	(21)	(22)
A_1	$\frac{1}{2}$			$\frac{1}{2}$
A_2		$\frac{1}{2}$	$-\frac{1}{2}$	
$(E)1$	$-\frac{1}{2}$			$\frac{1}{2}$
$(E)2$		$\frac{1}{2}$	$\frac{1}{2}$	

$E \times F_1$	(11)	(21)
$(F_1)1$	$-\frac{1}{4}$	$\frac{3}{4}$
$(F_2)1$	$-\frac{3}{4}$	$-\frac{1}{4}$

$E \times F_1$	(12)	(22)
$(F_1)2$	$-\frac{1}{4}$	$-\frac{3}{4}$
$(F_2)2$	$\frac{3}{4}$	$-\frac{1}{4}$

$E \times F_1$	(13)	(23)
$(F_1)3$	1	
$(F_2)3$		1

$E \times F_2$	(11)	(21)
$(F_1)1$	$-\frac{3}{4}$	$-\frac{1}{4}$
$(F_2)1$	$-\frac{1}{4}$	$\frac{3}{4}$

$E \times F_2$	(12)	(22)
$(F_1)2$	$\frac{3}{4}$	$-\frac{1}{4}$
$(F_2)2$	$-\frac{1}{4}$	$-\frac{3}{4}$

$E \times F_2$	(13)	(23)
$(F_1)3$		1
$(F_2)3$	1	

$F_i \times F_i$	(11)	(22)	(33)
A_1	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$
$(E)1$	$-\frac{1}{6}$	$-\frac{1}{6}$	$\frac{2}{3}$
$(E)2$	$\frac{1}{2}$	$-\frac{1}{2}$	0

$i = 1, 2.$

$F_i \times F_i$	(23)	(32)
$(F_1)1$	$\frac{1}{2}$	$-\frac{1}{2}$
$(F_2)1$	$\frac{1}{2}$	$\frac{1}{2}$

$F_i \times F_i$	(13)	(31)
$(F_1)2$	$-\frac{1}{2}$	$\frac{1}{2}$
$(F_2)2$	$\frac{1}{2}$	$\frac{1}{2}$

$F_i \times F_i$	(12)	(21)
$(F_1)3$	$\frac{1}{2}$	$-\frac{1}{2}$
$(F_2)3$	$\frac{1}{2}$	$\frac{1}{2}$

8.9. Molecular Orbital Theory

1. A molecule is a many–electron system. One of the successful theories in describing molecules is the so–called *molecular orbital theory.* The essence of the theory is as follows: Suppose that there is a molecule consisting of n atoms. Let us first strip several, say n, electrons off the

molecule and then consider a single electron moving around the molecular skeleton — an n-valent ion. The possible states of a single electron in the skeleton are called *molecular orbitals.*

Let $\mathbf{R}_i, i = 1, 2, \ldots, n$ be the position vectors of the n nuclei and $\mathbf{r}$ be the position vector of the electron, as shown in Fig. 8.9. Suppose that $\phi^l_{\lambda_2\mu_2}$ is the atomic orbital wave function (single electron wave function) in the $O_3 \supset G \supset G(s)$ classification. The approximation obtained by choosing linear combinations of the n atomic orbitals as the molecular orbitals,

$$\psi = \sum_{i=1}^{n} \sum_{\mu_2} b_{\mu_2 i} \phi^l_{\lambda_2\mu_2}(i) \ , \quad \phi^l_{\lambda_2\mu_2}(i) \equiv \phi^l_{\lambda_2\mu_2}(\mathbf{r} - \mathbf{R}_i) \ , \tag{8-78}$$

is called the atomic orbital linear combination approximation for molecular orbitals. Equation (8-78) shows that the electron is not localized to a particular nucleus. Obviously ψ must be an irreducible basis $(\lambda)\mu$ of the point group G of the molecule,

$$\psi^{(\lambda)\tau}_{\mu} = \sum_{\mu_2 i} b^{(\lambda)\tau}_{\mu,\mu_2 i} \phi^l_{\lambda_2\mu_2}(\mathbf{r} - \mathbf{R}_i) \ , \tag{8-79}$$

where τ is a multiplicity label. The last result is called *symmetry adapted linear combination* (SALC), or the *single electron SALC.*

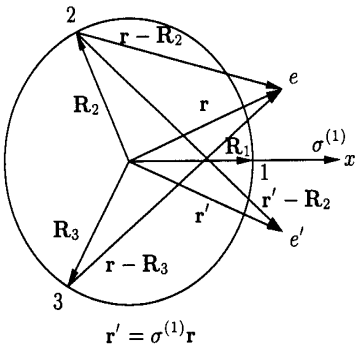


Fig. 8.9. Electron and nuclei positions.

2. The SALC (8-79) is not yet a molecular orbital wave function. We have to consider interactions between various atomic orbitals, that is, diagonalize the single electron Hamiltonian H in the basis (8-79). The molecular orbital wave function $\psi^{(\lambda)}_{\mu}(E)$ with energy E is a linear combination of $\psi^{(\lambda)\tau}_{\mu}$ in (8-79),

$$\psi^{(\lambda)}_{\mu}(E) = \sum_{\tau} a_{E,\tau} \psi^{(\lambda)\tau}_{\mu} \ . \tag{8-80a}$$

According to (3-334c) the expansion coefficients $a_{E,\tau}$ satisfy the eigenequation

$$\sum_{\tau'} \left[\langle \psi^{(\lambda)\tau}_{\mu} | H | \psi^{(\lambda)\tau'}_{\mu} \rangle - \delta_{\tau\tau'} E \right] a_{E,\tau'} = 0 \ , \tag{8-80b}$$

where the quantum number μ can be taken any possible value.

3. Many compounds, such as the metal complexes, have a metal atom in the center and several equivalent atoms, called *ligands*, surrounding the center. In such cases, the first step in constructing the SALC is to linearly combine the orbitals of the surrounding atoms into the $G \supset G(s)$ irreducible bases (that is, the SALC). The second step is to find the $O_3 \supset G \supset G(s)$

irreducible basis for the central atom. Finally, one considers the interaction among the various atomic orbitals, namely, linearly combine the SALC (possible more than one) of the surrounding atoms and the wave function of the central atom, all belonging to the same irrep λ. By solving the secular equation, we can obtain the molecular orbitals. An electron in any molecular orbital belongs to the surrounding atoms as well as to the central atom.

4. Having found the molecular orbitals, we now return the n electrons which were originally stripped off, to the molecular orbitals according to the ordering of the energy levels. Each energy level can accommodate at most $2h_\lambda$ electrons, where the factor 2 comes from the two possible spin states of the electron. Each possible way of filling the molecular orbitals is called a configuration. The configuration with the lowest orbitals all occupied is called the ground state configuration. The others are called excited configurations. One configuration may correspond to several n–electron product wave functions.

5. Linearly combine these n–electron product wave functions into the $G \supset G(s)$ irreducible basis $\Phi_\mu^{(\lambda)\beta}$, called the *many–electron SALC*, β being the additional quantum numbers. $\Psi_\mu^{(\lambda)\beta}$ is an approximate molecule wave function, corresponding to the extreme single particle model in nuclear physics.

6. Furthermore, one can consider the interaction between the electrons. By diagonalizing the Hamiltonian in the basis $\Psi_\mu^{(\lambda)\beta}$ with the same λ and μ but different β (notice that β includes the configuration label), we can obtain a better approximation to the molecular wave functions. This corresponds to the configuration interaction approximation in atomic or nuclear physics.

From the above discussions, we see that the molecular orbital theory is very close to the atomic or nuclear shell model and is thus sometimes called the *molecular shell model.* A more detailed discussion of point (5) will be given in Sections 9.11.

8.10. Single Electron SALC

Let us first consider the case when all the atomic orbitals are s orbitals (so that $l = 0$). Suppose that S is an element of the group G. From (2-58) we have

$$\begin{aligned} S\varphi(i) &= S\varphi(\mathbf{r} - \mathbf{R}_i) = \varphi(S^{-1}\mathbf{r} - \mathbf{R}_i) = \varphi(S^{-1}(\mathbf{r} - S\mathbf{R}_i)) \\ &= \varphi(\mathbf{r} - S\mathbf{R}_i) = \varphi(\mathbf{r} - \mathbf{R}_j) = \varphi(j) \ , \end{aligned} \tag{8-81}$$

where we have used the fact that the s orbital wave function depends on only the length of $\mathbf{r} - \mathbf{R}_i$, $\varphi(\mathbf{r} - \mathbf{R}_i) = \varphi(|\mathbf{r} - \mathbf{R}_i|)$. $\mathbf{R}_j = S\mathbf{R}_i$ is the position vector resulting from applying the operator S to the position vector $\mathbf{R}_i$ and is the position vector of the vertex j. From (8-81) it is seen that under the group operations, the s–state atomic orbitals $\varphi(i)$ transform as the vertices. For example, in Fig. 8.9, under the reflection $\sigma^{(1)}$, $\varphi(2)$ goes over to $\varphi(3)$,

$$\begin{aligned} \sigma^{(1)}\varphi(2) &= \sigma^{(1)}\varphi(\mathbf{r} - \mathbf{R}_2) = \varphi(\mathbf{r}' - \mathbf{R}_2) \\ &= \varphi(\sigma^{(1)}(\mathbf{r} - \sigma^{(1)}\mathbf{R}_2)) = \varphi(\mathbf{r} - \mathbf{R}_3) = \varphi(3) \ . \end{aligned} \tag{8-82}$$

Assume that under the operation S, the vertex i goes over to j and let

$$D_{ki}(S) = \delta_{kj} \ . \tag{8-83}$$

Thus

$$S\varphi(i) = \sum_k D_{ki}(S)\varphi(k) \ . \tag{8-84}$$

Due to the overlap between atomic orbitals, the $\varphi(i)$ are not orthogonal ,

$$g_{ij} = \langle\varphi(i)|\varphi(j)\rangle \neq \delta_{ij} \ . \tag{8-85}$$

In quantum chemistry, the overlap integrals g_{ij} (that is, the metric tensor) are usually designated S_{ij}. The metric tensor g_{ij} becomes δ_{ij} only when the atoms i and j are infinitely far apart from each other. According to (2-15), we can introduce the dual basis $\{\overline{\varphi}(i)\}$. The quantity $D_{ki}(S)$ in (8-84) can be written as

$$D_{ki}(S) = \langle \overline{\varphi}(k) | S | \varphi(i) \rangle \ . \tag{8-86}$$

Using the isomorphism between a point group and a subgroup of the permutation group (such as Eq. (3-21) for the group $\mathcal{C}_{6v}$, Table 8.2-2 for T_d and O, respectively), it is very easy to find $D_{ki}(S)$. Examples will be given later.

Since $\{\varphi(i)\}$ is not in general an orthogonal basis, the rep carried by it is not in general unitary (see (2-121a)). However, the rep given by (8-83) or (8-86) is still unitary,

$$D_{ij}(S^{-1}) = D_{ji}(S) = D^{\dagger}_{ij}(S) \ . \tag{8-87}$$

Diagonalizing the CSCO–II of G in the basis $\{\varphi(i)\}$ gives the irreducible basis of G,

$$\psi^{(\lambda)\tau}_{\mu} = \sum_i u^{(\lambda)\tau}_{\mu,i} \varphi(i) \ , \tag{8-88}$$

while the coefficients $u^{(\lambda)\tau}_{\mu,i}$ are determined by the eigenequations

$$\sum_i \left[\left\langle \overline{\varphi}(j) \left| \begin{matrix} C \\ C(s) \end{matrix} \right| \varphi(i) \right\rangle - \binom{\lambda}{\mu} \delta_{ij} \right] u^{(\lambda)\tau}_{\mu,i} = 0 \ . \tag{8-89}$$

Suppose that the overlaps between the atomic orbitals $\{\varphi(i)\}$ are negligible, that is,

$$\overset{\circ}{g}_{ij} = \langle \overset{\circ}{\varphi}(i) | \overset{\circ}{\varphi}(j) \rangle = \delta_{ij} \ . \tag{8-90}$$

In such a case, the SALC would be

$$\overset{\circ}{\psi}{}^{(\lambda)\tau}_{\mu} = \sum_i a^{(\lambda)\tau}_{\mu,i} \overset{\circ}{\varphi}(i) \ , \tag{8-91}$$

where $a^{(\lambda)\tau}_{\mu,i}$ is a unitary matrix. According to Sec. 3.14, the coefficients $u^{(\lambda)\tau}_{\mu,i}$ and $a^{(\lambda)\tau}_{\mu,i}$ differ only by a multiplicative factor, $N^{(\lambda)\tau}_{\mu}$. Therefore

$$\psi^{(\lambda)\tau}_{\mu} = N^{(\lambda)\tau}_{\mu} \sum_i a^{(\lambda)\tau}_{\mu,i} \varphi(i) \ , \tag{8-92}$$

$$N^{(\lambda)\tau}_{\mu} = \left(\sum_{ij} a^{(\lambda)\tau^*}_{\mu,j} g_{ij} a^{(\lambda)\tau}_{\mu,j} \right)^{-1/2} \ .$$

In the following, for simplicity, we assume that $g_{ij} = \delta_{ij}$, that is we let

$$\psi^{(\lambda)\tau}_{\mu} = \sum_i a^{(\lambda)\tau}_{\mu,i} \varphi(i) \ . \tag{8-93}$$

To return to the non–orthogonal basis $\{\varphi(i)\}$, all we need to do is to multiply the right–hand side of (8-93) by the coefficients $N^{(\lambda)\tau}_{\mu}$.

The method for finding the irreducible basis of the permutation group can be used for finding the SALC (8-93).

Example 1: The group $\mathcal{C}_{3v}$. From the isomorphism (1-15) between the group $\mathcal{C}_{3v}$ and the permutation group S_3, according to (3-82) and (3-90), we can write down the eigenfunctions of $3\sigma = \sigma^{(1)} + \sigma^{(2)} + \sigma^{(3)}$, and $\sigma^y = \sigma^{(1)}$, that is, the $\mathcal{C}_{3v} \supset \mathcal{C}_s$ irreducible basis,

$$\psi^{A_1} = \tfrac{1}{\sqrt{3}}[\varphi(1) + \varphi(2) + \varphi(3)]N^{A_1} , \tag{8-94}$$

$$\psi_1^E = \tfrac{1}{\sqrt{6}}[2\varphi(1) - \varphi(2) - \varphi(3)]N_1^E ,$$

$$\psi_2^E = \tfrac{1}{\sqrt{2}}[\varphi(2) - \varphi(3)]N_2^E . \tag{8-95}$$

Example 2: The group T_d. From Table 8.2-2 we can find the operation of the CSCO–II, $(6S_4, S_{4z}^-)$, of T_d on the function $\varphi(i)$,

$$\begin{aligned} &C\varphi(i) = 2\big(\varphi(j) + \varphi(k) + \varphi(l)\big) , \qquad \text{cyclic in } i,j,k,l = 1,2,3,4 , \\ &S_{4z}^-\varphi(1) = \varphi(3), \quad S_{4z}^-\varphi(2) = \varphi(4), \quad S_{4z}^-\varphi(3) = \varphi(2), \quad S_{4z}^-\varphi(4) = \varphi(1) . \end{aligned} \tag{8-96}$$

Solving the eigenequation of (C, S_{4z}^-), we get the irreducible bases,

$$\begin{aligned} \psi^{A_1} &= \psi^{(6)} = \tfrac{1}{2}[\varphi(1) + \varphi(2) + \varphi(3) + \varphi(4)] , \\ \psi_3^{F_2} &= \psi_{-1}^{(-2)} = \tfrac{1}{2}[\varphi(1) + \varphi(2) - \varphi(3) - \varphi(4)] . \end{aligned} \tag{8-97a}$$

From (8-42) and Table 8.2-2 we obtain the two other components of the irrep F_2,

$$\begin{aligned} \psi_1^{F_2} &= (23)\psi_3^{F_2} = \tfrac{1}{2}[\varphi(1) - \varphi(2) + \varphi(3) - \varphi(4)] , \\ \psi_2^{F_2} &= (24)\psi_3^{F_2} = \tfrac{1}{2}[\varphi(1) - \varphi(2) - \varphi(3) + \varphi(4)] . \end{aligned} \tag{8-97b}$$

We now introduce another method given by Fieck (1977) for finding the coefficients $a_{\mu,i}^{(\lambda)}$ in (8-93). Fieck proved that apart from normalization factors, there is a simple relation between the values of the $O_3 \supset G \supset G(s)$ irreducible basis at the vertex i, $\phi_{\lambda\mu}^l(\mathbf{R}_i)$, and the coefficient $a_{\mu,i}^{(\lambda)}$,

$$a_{\mu,i}^{(\lambda)l} = \phi_{\lambda\mu}^{(l)}(\mathbf{R}_i) , \tag{8-98}$$

where $\mathbf{R}_i$ is the position vector of the vertex i. The multiplicity τ is larger than one if different choices of l on the right–hand side of (8-98) lead to different values of $a_{\mu,i}^{(\lambda)l}$. In such cases, l can serve as the multiplicity label. Needless to say, to find $a_{\mu,i}^{(\lambda)l}$ from (8-98), it is most convenient to choose l as small as possible. Before proving (8-98) we need another result.

From our assumption, $\phi_{\lambda\mu}^l$ transform according to the irrep $D^{(\lambda)}$ under the point group G,

$$S\phi_{\lambda\mu}^{(l)}(\mathbf{r}) = \sum_{\mu'} D_{\mu'\mu}^{(\lambda)}(S)\phi_{\lambda\mu'}^{(l)}(\mathbf{r}) . \tag{8-99}$$

Letting $\mathbf{r} = \mathbf{R}_j$, we get

$$S\phi_{\lambda\mu}^{(l)}(\mathbf{R}_j) = \sum_{\mu'} D_{\mu'\mu}^{(\lambda)}(S)\phi_{\lambda\mu'}^{(l)}(\mathbf{R}_j) . \tag{8-100}$$

On the other hand, using (8-84) and noting that the D in (8-84) is a real and symmetric matrix, the left–hand side of (8-100) can be put into the following form,

$$S\phi_{\lambda\mu}^{(l)}(\mathbf{R}_j) = \phi_{\lambda\mu}^{(l)}\Big(\sum_i D_{ij}(S^{-1})\mathbf{R}_i\Big) = \sum_i D_{ji}(S)\phi_{\lambda\mu}^{(l)}(\mathbf{R}_i) . \tag{8-101}$$

Comparing (8-100) with (8-101), we have

$$\sum_{\mu'} D_{\mu'\mu}^{(\lambda)}(S)\phi_{\lambda\mu'}^{(l)}(\mathbf{R}_j) = \sum_i D_{ji}(S)\phi_{\lambda\mu}^{(l)}(\mathbf{R}_i) . \tag{8-102}$$

It is this relation that we will use below for proving (8-98).

To prove (8-98), it suffices to show that

$$\psi_{\mu}^{(\lambda)l}(\mathbf{r}) = N \sum_{i} \phi_{\lambda\mu}^{(l)}(\mathbf{R}_i)\varphi(i) \tag{8-103}$$

is the $G \supset G(s)$ irreducible basis $(\lambda)\mu$, where N is a normalization constant. Noting that $\phi_{\lambda\mu}^{l}(\mathbf{R}_i)$ in (8-103) are coefficients and the group operation S only effects the function $\varphi(i)$, and using (8-102) we get

$$\begin{aligned} S\psi_{\mu}^{(\lambda)l}(\mathbf{r}) &= N \sum_{ij} \phi_{\lambda\mu}^{(l)}(\mathbf{R}_i) D_{ji}(S)\varphi(j) \\ &= N \sum_{\mu' j} D_{\mu'\mu}^{(\lambda)}(S)\phi_{\lambda\mu'}^{(l)}(\mathbf{R}_j)\varphi(j) = \sum_{\mu'} D_{\mu'\mu}^{(\lambda)}(S)\psi_{\mu'}^{(\lambda)l}(\mathbf{r}) \ . \end{aligned} \tag{8-104}$$

It should be stressed that for cases with multiplicities, the functions in Eq. (8-103) with different l are not orthogonal.

Example 3: The group C_{3v} and T_d. According to the coordinates of the vertices in Fig 8.9 and in Fig. 8.2-3, we obtain the values of x, y, and z listed in Tables 8.10-1 and 8.10-2, respectively. From (3-78) and Table 8.6-2 we get the $O_3 \supset G \supset G(s)$ irreducible basis $\phi_{\lambda\mu}^{l}(\mathbf{r})$. Then letting $\mathbf{r} = \mathbf{R}_1, \mathbf{R}_2, \ldots$, we obtain the values of $\phi_{\lambda\mu}^{l}(\mathbf{R}_i)$ listed in Tables 8.10-1 and 8.10-2.

Table 8.10-1. The values of $\phi_{\lambda\mu}^{l}(\mathbf{R}_i)$ for the group C_{3v}.

$\phi_{\lambda\mu}^{(l)}(\mathbf{r})$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$
$\phi^{A} = x^2 + y^2$	1	1	1
$\phi_{E,1}^{l=1} = x$	1	$-\frac{1}{2}$	$-\frac{1}{2}$
$\phi_{E,2}^{l=1} = y$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$
$\phi_{E,1}^{l=2} = x^2 - y^2$	1	$-\frac{1}{2}$	$-\frac{1}{2}$
$\phi_{E,2}^{l=2} = -2xy$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$

Table 8.10-2. The values of $\phi_{\lambda\mu}^{l}(\mathbf{R}_i)$ for the group T_d.

$\phi_{\lambda\mu}^{(l)}(\mathbf{r})$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}_4$
$\phi_{A_1} = x^2 + y^2 + z^2$	3	3	3	3
$\phi_{F_2,1}^{l=1} = x$	1	−1	1	−1
$\phi_{F_2,2}^{l=1} = y$	1	−1	−1	1
$\phi_{F_2,3}^{l=1} = z$	1	1	−1	−1

Comparing Table 8.10-1 with Eq. (8-95), and Table 8.10-2 with Eq. (8-97), one sees that the EFM and Eq. (8-98) give identical results (including the phase). In Table 8.10-1, we deliberately listed the values of $\phi_{\lambda\mu}^{l=1}$ as well as $\phi_{\lambda\mu}^{l=2}$. That they lead to the same values of $\phi_{\lambda\mu}^{l}(\mathbf{R}_i)$ shows that here the irrep E occurs only once.

Now we consider the cases where $l \neq 0$.

Suppose that the atomic orbital wave function $\phi_{\lambda_2\mu_2}^{l_2}(i) = \phi_{\lambda_2\mu_2}^{l_2}(\mathbf{r} - \mathbf{R}_i)$ belongs to the irreps l_2, λ_2, μ_2 of the group chain $O_3 \supset G \supset G(s)$. Let us first consider the action of the group elements S on the function

$$\begin{aligned} S\phi_{\lambda_2\mu_2}^{l_2}(i) &= \phi_{\lambda_2\mu_2}^{l_2}(S^{-1}\mathbf{r} - \mathbf{R}_i) = \phi_{\lambda_2\mu_2}^{l_2}(S^{-1}(\mathbf{r} - S\mathbf{R}_i)) \\ &= \sum_{\mu_2'} D_{\mu_2'\mu_2}^{(\lambda_2)}(S)\phi_{\lambda_2\mu_2'}^{l_2}(\mathbf{r} - S\mathbf{R}_i) \\ &= \sum_{\mu_2'} D_{\mu_2'\mu_2}^{(\lambda_2)}(S)\phi_{\lambda_2\mu_2'}^{l_2}(\mathbf{r} - \sum_{j} D_{ji}(S)\mathbf{R}_j) \ . \end{aligned} \tag{8-105}$$

Since in (8-105) there is only one non–vanishing term in the summation over j, the summation symbol can be shifted to the left,

$$S\phi^{l_2}_{\lambda_2\mu_2}(i) = \sum_{j\mu_2'} D^{(\lambda_2)}_{\mu_2'\mu_2}(S) D_{ji}(S) \phi^{l_2}_{\lambda_2\mu_2'}(j) \ . \tag{8-106}$$

This shows that $\phi^{l_2}_{\lambda_2\mu_2}(i)$ transform according to $D^{(\lambda_2)} \otimes D$ under the group G.

Introducing

$$\varphi_{\lambda_1\mu_1,\lambda_2\mu_2} = \sum_i \phi^{l_1}_{\lambda_1\mu_1}(\mathbf{R}_i) \phi^{l_2}_{\lambda_2\mu_2}(i) \ , \tag{8-107}$$

and using (8-102) and (8-106), we obtain

$$\begin{aligned} S\varphi_{\lambda_1\mu_1,\lambda_2\mu_2} &= \sum_{ij\mu_2'} \phi^{l_1}_{\lambda_1\mu_1}(\mathbf{R}_i) D^{(\lambda_2)}_{\mu_2'\mu_2}(S) D_{ji}(S) \phi^{l_2}_{\lambda_2\mu_2'}(j) \\ &= \sum_{\mu_2'\mu_1' j} D^{(\lambda_1)}_{\mu_1'\mu_1}(S) D^{(\lambda_2)}_{\mu_2'\mu_2}(S) \phi^{l_1}_{\lambda_1\mu_1'}(\mathbf{R}_j) \phi^{l_2}_{\lambda_2\mu_2'}(j) \\ &= \sum_{\mu_2'\mu_1'} D^{(\lambda_1)}_{\mu_1'\mu_1}(S) D^{(\lambda_2)}_{\mu_2'\mu_2}(S) \varphi_{\lambda_1\mu_1',\lambda_2\mu_2'} \ . \end{aligned} \tag{8-108}$$

Therefore, under the group $G, \varphi_{\lambda_1\mu_1,\lambda_2\mu_2}$ transforms according to $D^{(\lambda_1)} \otimes D^{(\lambda_2)}$. Using the CG coefficients of the point group, we can find the SALC

$$\psi^{(\lambda)\tau}_{\mu} = \sum_{\mu_1\mu_2} C^{(\lambda)\theta,\mu}_{\lambda_1\mu_1,\lambda_2\mu_2} \varphi_{\lambda_1\mu_1,\lambda_2\mu_2} \ , \tag{8-109a}$$

that is,

$$\psi^{(\lambda)\tau}_{\mu}(\mathbf{r}) = N \sum_{\mu_1\mu_2 i} C^{(\lambda)\theta,\mu}_{\lambda_1\mu_1,\lambda_2\mu_2} \phi^{l_1}_{\lambda_1\mu_1}(\mathbf{R}_i) \phi^{l_2}_{\lambda_2\mu_2}(\mathbf{r} - \mathbf{R}_i) \ , \tag{8-109b}$$

where N is a normalization factor and τ is the multiplicity label,

$$\tau = \lambda_1, \lambda_2, \theta, l_1 \ . \tag{8-110}$$

The choice of l_1 was discussed after Eq. (8-98). Comparing (8-79) and (8-109), we find that the coefficients in (8-79) are

$$b^{(\lambda)\tau}_{\mu,\mu_2 i} = N \sum_{\mu_1} C^{(\lambda)\theta,\mu}_{\lambda_1\mu_1,\lambda_2\mu_2} \phi^{l_1}_{\lambda_1\mu_1}(\mathbf{R}_i) \ . \tag{8-111}$$

When λ_2 is one–dimensional, (8-109b) reduces to

$$\begin{aligned} \psi^{(\lambda)\tau}_{\mu}(\mathbf{r}) &= N \sum_i \phi^{l_1}_{\lambda_1\mu_1}(\mathbf{R}_i) \phi^{l_2}_{\lambda_2}(\mathbf{r} - \mathbf{R}_i) \, , \\ (\lambda) &= (\lambda_1) \times (\lambda_2) \ . \end{aligned} \tag{8-112}$$

When (λ_2) is an identity rep, (8-109b) or (8-112) reduces to (8-103).

Example 4: The group T_d for the p atomic orbitals. Suppose that the four equivalent atomic orbitals are p orbitals. The p_x, p_y and p_z orbital wave functions are proportional to x, y and z, respectively. According to Table 8.6-2, they belong to the irrep F_2 of the group T_d. Therefore, in (8-109b) we should let $\{\phi^{l_2}_{\lambda_2\mu_2}(i)\} = \{\phi^{(p)}_{F_2\mu_2}(i)\} = \{x(i), y(i), z(i)\}$. From (8-109b), Table 8.10-2 and Table 8.8-2, we obtain the SALC for the p orbital of the group T_d, as listed in Table 8.10-3.

Table 8.10-3. SALC's for the p orbitals of T_d.
$|(\lambda_1\lambda_2)\lambda,\mu\rangle = N\sum_{\mu_1\mu_2 i} C^{\lambda,\mu}_{\lambda_1\mu_1,\lambda_2\mu_2}\phi^{l_1=1}_{\lambda_1\mu_1}(\mathbf{R}_i)\phi^{l_2=1}_{\lambda_2\mu_2}(i)$.

$(\lambda_1,\lambda_2)\lambda,\mu$	$x(1)$	$x(2)$	$x(3)$	$x(4)$	$y(1)$	$y(2)$	$y(3)$	$y(4)$	$z(1)$	$z(2)$	$z(3)$	$z(4)$
$(F_2,F_2)A_1$	$\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$	$\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$	$\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$	$\frac{1}{\sqrt{12}}$	$\frac{1}{\sqrt{12}}$	$\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$	$-\frac{1}{\sqrt{12}}$
$(F_2,F_2)E,1$	$-\frac{1}{\sqrt{24}}$	$\frac{1}{\sqrt{24}}$	$-\frac{1}{\sqrt{24}}$	$\frac{1}{\sqrt{24}}$	$-\frac{1}{\sqrt{24}}$	$\frac{1}{\sqrt{24}}$	$\frac{1}{\sqrt{24}}$	$-\frac{1}{\sqrt{24}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$
$E,2$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$				
$(F_2,F_2)F_1,2$					$-\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$
$F_1,2$	$\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$					$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$
$F_1,3$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$				
$(F_2,F_2)F_2,1$					$\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$
$F_2,2$	$\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$					$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$
$F_2,3$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	$-\frac{1}{\sqrt{8}}$				
$(A_1,F_2)F_2,1$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$								
$F_2,2$					$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$				
$F_2,3$									$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$

Equation (8-109b) gives a general method for finding the single electron SALC. It is most suitable for the cases with high l atomic orbitals. However, for some simple cases, it is more convenient to use the projection operator method, as shown below.

1) The group $\mathcal{C}_n(\mathcal{C}_{nh})$. Suppose that n equivalent atoms sit on the vertices of a regular n–sided polygon, such as the n carbon atoms in the molecule C_nH_n, with each carbon atom contributing one s or p_z orbital $\varphi(i)$.

Applying the projection operator P^μ in (8-37a) to any atomic orbital, say $\varphi(1)$, and using

$$C_n\varphi(1) = \varphi(2), \quad C_n^k\varphi(1) = \varphi(k+1)\ , \tag{8-113}$$

with the convention $\varphi(n+1) \equiv \varphi(1)$, we find the irreducible basis of $\mathcal{C}_n$ to be

$$\psi^{(\mu)} = \sqrt{\frac{1}{n}}\sum_{k=1}^{n} e^{i(k-1)\mu\beta}\varphi(k)\ , \tag{8-114}$$
$$\beta = \tfrac{2\pi}{n}, \mu = 0, \pm1, \pm2, \ldots, \pm\left[\tfrac{n}{2}\right]\ .$$

2) The group $D_n(D_{nh})$.

Suppose that the atom 1 is on the x axis, therefore

$$C_{2x}\varphi(1) = \xi\varphi(1)\ , \tag{8-115}$$

where $\xi = 1(-1)$ for $s(p_z)$ orbital. Also suppose that we need to find the $D_n \supset \mathcal{C}_{2x}$ real basis functions. For this purpose it is most convenient to use the $D_n \supset \mathcal{C}_{2x}, \bar{D}_n \supset \bar{\mathcal{C}}_n$ generalized projection operator instead of the $D_n \supset \mathcal{C}_{2x}$ conventional projection operator. Applying (8-37c) and (8-39a) to $\varphi(1)$ and using (8-115) we have

$$\psi^{A_{\rho\xi}} = \sqrt{\frac{1}{n}}\sum_{k=1}^{n} \rho^{k-1}\varphi(k)\ , \tag{8-116}$$

where $\rho = \pm 1$ for even n and $\rho = 1$ for odd n, and

$$\psi_{\pm 1}^{E_\mu} = \frac{1}{\sqrt{2}}\left[\psi^{(\mu)} \pm \xi\psi^{(\mu)*}\right] , \quad \mu > 0. \tag{8-117}$$

It is seen that basis vectors of the two-dimensional irrep E_μ of D_n or D_{nh} can be found from the real and imaginary part of the irreducible basis vectors $\psi^{(\mu)}$ of C_n. For p_z orbital with $\xi = -1$ we have

$$\begin{aligned} \psi_1^{E_\mu} &= -\sqrt{\frac{2}{n}}\sum_{k=1}^{n} \sin\big((k-1)\mu\beta\big)\varphi(k) , \\ \psi_{-1}^{E_\mu} &= \sqrt{\frac{2}{n}}\sum_{k=1}^{n} \cos\big((k-1)\mu\beta\big)\varphi(k) , \end{aligned} \qquad \mu = 1, 2, \ldots, \left[\tfrac{n}{2}\right] . \tag{8-118}$$

For example, letting $\xi = -1, n = 6, \beta = 60°$, we have the D_{6h} SALC of p_z electron,

$$\begin{aligned} \psi^{A_{2u}} &= \sqrt{\frac{1}{6}}\sum_{i=1}^{6}\varphi(i) , \\ \psi^{B_{1g}} &= \sqrt{\frac{1}{6}}[\varphi(1) - \varphi(2) + \varphi(3) - \varphi(4) + \varphi(5) - \varphi(6)] , \\ \psi_1^{E_{1g}} &= -\frac{1}{2}[\varphi(2) + \varphi(3) - \varphi(5) - \varphi(6)] , \\ \psi_{-1}^{E_{1g}} &= \sqrt{\frac{1}{12}}[2\varphi(1) + \varphi(2) - \varphi(3) - 2\varphi(4) - \varphi(5) + \varphi(6)] , \\ \psi_1^{E_{2u}} &= -\frac{1}{2}[\varphi(2) - \varphi(3) + \varphi(5) - \varphi(6)] , \\ \psi_{-1}^{E_{2u}} &= \sqrt{\frac{1}{12}}[2\varphi(1) - \varphi(2) - \varphi(3) + 2\varphi(4) - \varphi(5) - \varphi(6)] . \end{aligned} \tag{8-119}$$

Though the SALC is a drastic simplification of the real case, it is still not easy to use (8-80b) to find molecular orbitals. Further approximations are needed. The crudest one is the *Hückel approximation*, which can be expressed in terms of three approximations:

1. The atomic orbital are orthogonal,

$$g_{ij} = \langle\varphi(i)|\varphi(j)\rangle = \delta_{ij} .$$

2. The diagonal elements of H are equal to a constant,

$$\langle\varphi(i)|H|\varphi(i)\rangle = E_0 .$$

3. Only the off-diagonal elements of H between the neighboring atomic orbitals are non-zero, and they are equal to $-F$,

$$\langle\varphi(i)|H|\varphi(j)\rangle = \begin{cases} -F & \text{when } i \text{ and } j \text{ are neighboring orbitals} , \\ 0 & \text{otherwise} , \end{cases}$$

where the constant $F > 0$.

The Hückel approximation is a very crude one. Nevertheless, it has met with success. Though it is not reliable quantitatively, it often gives correct qualitative results.

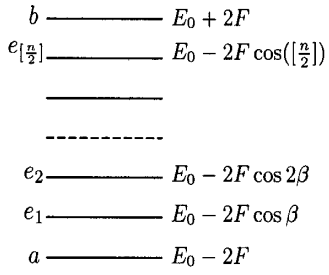


Fig. 8.10-1. The energy levels for molecular orbitals of $D_{nh}, \beta = 2\pi/n$.

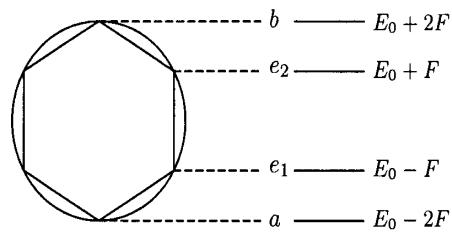


Fig. 8.10-2. The energy levels for molecular orbitals of D_{6h}.

Example 1: Find the energy levels of the molecule C_nH_n. From (8-118) and (3-221c)

$$\begin{aligned} E_\mu &= \frac{2}{n}\left\langle \sum_{k=1}^{n} \sin\big((k-1)\mu\beta\big)\varphi(k)\Big|H\Big|\sum_{k'=1}^{n}\sin((k'-1)\mu\beta)\varphi(k')\right\rangle \\ &= E_0 - \frac{4}{n}F\sum_{k=1}^{n}\sin((k-1)\mu\beta)\sin(k\mu\beta) \\ &= E_0 - 2F\cos(\mu\beta)\ . \end{aligned} \tag{8-120}$$

The energy levels of (8-120) for D_{nh} molecular orbitals are shown in Fig. 8.10-1, while those for D_{6h} are shown in Fig. 8.10-2. In these diagrams, the small letters denote the irrep labels.

There is a simple method for drawing such energy level diagrams: Draw a regular polygon with n sides, as shown in Fig. 8.10-2. Then the lines connecting the two vertices on the same level give the energy levels.

Bonding orbitals are the orbitals with energies less than E_0. Thus for D_{6h}, the one-dimensional orbital a and the two-dimensional orbital e_1 are bound orbitals. It is favorable in energy for electrons to occupy those bond orbitals. Similarly *anti-bonding orbitals* are the orbitals with energies greater than E_0, such as the orbitals e_2 and b in Fig. 8.10-2.

Example 2: The ground state energy of the benzene molecule. Figure 8.10-2 gives the energy levels of a single electron moving around a benzene molecule with six electrons stripped off. Let us now put the six electrons on the lowest orbitals in Fig. 8.10-1 and obtain the ground state configuration $(a)^2(e_1)^4$. The energy of the ground state is

$$E_g = 2(E_0 - 2F) + 4(E_0 - F) = 6E_0 - 8F\ .$$

We see that the energy is lowered by the amount $8F$ due to the interaction between the atomic orbitals. This is why the benzene molecule is very stable.

Example 3: The naphthalene molecule. The naphthalene molecule has the symmetry D_{2h}, as shown in Fig. 8.10-3. Each atom at a vertex contributes one p_z orbital. It is readily seen that under the group D_{2h}, the atomic orbitals $\varphi(1), \varphi(2), \ldots, \varphi(10)$ can be divided into three sets, $(\varphi(1), \varphi(4), \varphi(5), \varphi(8))$, $(\varphi(2), \varphi(3), \varphi(6), \varphi(7))$ and $(\varphi(9), \varphi(10))$, each transforming among themselves. According to Table 8.3-2, the CSCO of D_{2h} is (C_{2x}, C_{2y}, I). It is easy to find their simultaneous eigenfunctions, and the result is shown in Table 8.10-4.

Ex. 8.22. Using (8-116) and (8-118) construct the SALC of D_{5h}.

Ex. 8.23. Show that the SALC's for the group C_{nv} are given by (8-116) and (8-117) with $\xi = 1$.

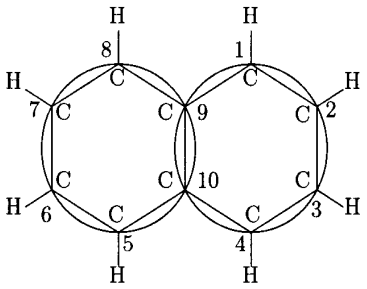


Fig. 8.10-3. The naphthalene molecule with the symmetry D_{2h}.

Table 8.10-4. The SALC for naphthalene $C_{10}H_8$.

C_{2x}	C_{2y}	I		$\varphi(2)$ $\varphi(1)$	$\varphi(3)$ $\varphi(4)$	$\varphi(6)$ $\varphi(5)$	$\varphi(7)$ $\varphi(8)$	$\varphi(9)$	$\varphi(10)$
-1	-1	-1	$\psi^{B_{1u}}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
1	1	-1	ψ^{A_u}	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$		
-1	1	1	$\psi^{B_{2g}}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$		
1	-1	1	$\psi^{B_{3g}}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$		
1	-1	1	$\psi^{B_{3g}}$					$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$
-1	-1	-1	$\psi^{B_{1u}}$					$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$

8.11. Double Point Groups and d–v Representations

8.11.1. The double point group method

In the previous sections, we considered only the single–valued reps of point groups. However, it is often necessary to take into account the spin degree of freedom of electrons if the spin–orbit coupling is not negligible. We then need to consider the spinor or double–valued reps of the point group, instead of the vector or single–valued reps. In Chapter 6 we introduced the double rotation group $SO_3^\dagger$ for obtaining the spinor reps of the rotation group. Similarly, we introduce the double point group $G^\dagger$.

Any point group is isomorphic either to a pure rotation point group, or to the direct product of a pure rotation point group and the inversion group (e, I). Consequently, it suffices to consider the double point group of the pure rotation group.

Corresponding to the point group

$$G = \{R_i : i = 1, 2, \ldots, |G|\} \ , \quad R_i = R_{\mathbf{n}_i}(\varphi_i) = R(\alpha_i\beta_i\gamma_i) \ , \tag{8-121a}$$

we have the double point group

$$G^\dagger = \{R_i, \tilde{R}_i : i = 1, 2, \ldots, |G|\} \ , \quad \tilde{R}_i = R_{\mathbf{n}_i}(\varphi_i + 2\pi) \ . \tag{8-121b}$$

The double point group is a subgroup of the double rotation group $SO_3^\dagger$ [(6-1d)]. The latter can also be expressed as

$$SO_3^\dagger = \{\pm D^{1/2}(\alpha\beta\gamma) : R(\alpha\beta\gamma) \in SO_3\} \ , \tag{8-121c}$$

while $G^\dagger$ as

$$G^\dagger = \{\pm D^{\frac{1}{2}}(\alpha_i\beta_i\gamma_i) : i = 1, 2, \ldots, |G|\} \ . \tag{8-121d}$$

8.11.2. Euler angles and group tables

Many of the methods of constructing double–valued representations of point groups rely on the formation of the double point group. The group table of $G^\dagger$ can be constructed in the following way: first determine the Euler angles α, β and γ for each element of the point group G; Then assign the matrices $\pm D^{\frac{1}{2}}(\alpha, \beta, \gamma)$ to the elements $(R, \tilde{R})$, and finally use matrix multiplication to get the group table of $G^\dagger$. However one could assign $R_i = D^{\frac{1}{2}}(\alpha, \beta, \gamma), \tilde{R}_i = -D^{\frac{1}{2}}(\alpha, \beta, \gamma)$, or $R_i = -D^{\frac{1}{2}}(\alpha, \beta, \gamma), \tilde{R}_i = D^{\frac{1}{2}}(\alpha, \beta, \gamma)$ with the consequences that the Euler–angle parameterization is not always unique in the spinor reps and inconsistency may occur in the multiplication relations of group elements. This is most easily seen in an example. The assignments on page 22 of Bradley & Cracknell (1972), $C_{4z} = D^{\frac{1}{2}}(0, 0, \frac{\pi}{2})$ and $C_{2z} = -D^{\frac{1}{2}}(0, 0, \pi)$, imply that $C_{4z} = \exp(-i\frac{\pi}{2}J_z), C_{2z} = -\exp(-i\pi J_z)$, rather than $C_{2z} = C_{4z}^2 = \exp(-i\pi J_z)$.

This non-uniqueness can be overcome by extending the domain of of the Euler angles from

$$0 \leq \alpha < 2\pi, \ 0 \leq \beta \leq \pi, \ 0 \leq \gamma < 2\pi,$$

to

$$0 \leq \alpha < 2\pi, \ 0 \leq \beta \leq \pi, \ 0 \leq \gamma < 4\pi \ .$$

By making the following assignment

$$R_i = D^{\frac{1}{2}}(\alpha_i, \beta_i, R_i), \ \tilde{R}_i = -D^{\frac{1}{2}}(\alpha_i, \beta_i, \gamma_i) \ , \tag{8-121e}$$

consistent group table can then be constructed for any double point group. The Euler angles in the extended domain for the groups $D_6^\dagger, O^\dagger, I^\dagger$ are listed in Fan, Chen, McAven & Butler (1999). The group table of $O^\dagger$ is given in Table 10.21-1, while the group table of $I^\dagger$ is available upon request. For s–v reps the group table of $O^\dagger$ in Table 10.21-1. is identical to Bradley & Cracknell's table.

As an simple example, the Euler angles of $D_2^\dagger$ and the multiplication table for $D_2^\dagger$ are given in Table 8.11-1. In that table we use $-R_i$ to denote $\tilde{R}_i$.

Table 8.11-1. Group multiplication table of $D_2^\dagger$.

	e	C_{2x}	C_{2y}	C_{2z}
	R_1	R_2	R_3	R_4
$(\alpha\beta\gamma)$:	(000)	$(0\pi\pi)$	$(0\pi 0)$	(00π)
$D^{1/2}(\alpha\beta\gamma)$:	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$
	1	2	3	4
	2	-1	4	-3
	3	-4	-1	2
	4	3	-2	-1

Remark 1: The $2|G|$ matrices in (8-121e) form the $SO_3 \downarrow G$ subduced representation $\frac{1}{2} \downarrow G$, which is two–dimensional and irreducible for any non–Abelian point group G, and is labelled as $E_{1/2}$. This irrep is called the *primitive* (Butler 1981) or *fundamental irrep* of G. It is "fundamental" in two senses: it serves, on one hand, as the defining matrix representation for

the group $G^{\dagger}$, and on the other hand, as the building block for constructing any irrep of G from the power of $E_{1/2}$, just as for the rotational group where any irreps can be built up from the fundamental irrep $j = 1/2$ by angular momentum addition.

Remark 2: From Table 8.11-1 it is seen that in the irrep $E_{1/2}$, the two–fold rotations C_{2m} are related to the Pauli matrices as $C_{2m} = -i\sigma_m$, $m = x, y, z$. Therefore in the spinor rep C_{2x} and C_{2y} anti–commute instead of commute. A general proof of this is given in (8-127a).

Remark 3: Note that (R_1, R_2, R_3, R_4) does not form a group. One quarter of the group table of $D_2^{\dagger}$ is enough. From that quarter one can easily form the other three quarters of the group table by inspection.

8.11.3. Some basic relations between point group operators

In Sec. 8.1 we obtained some relations for point group operators in the faithful reps of the groups, which are valid only for s–v reps. These relations are now extended so that they are valid for both s–v and d–v cases. For s–v (vector) and d–v (spinor) reps, the period of a rotation is 2π and 4π, respectively,

$$R_{\mathbf{n}}(2\pi) = \theta = \pm 1, \tag{8-122a}$$

where the index θ specifies the type (s–v or d–v) of the representations,

$$\theta = \begin{cases} 1, & \text{for s–v reps,} \\ -1, & \text{for d–v reps.} \end{cases} \tag{8-122b}$$

The operator for a rotation about the axis $\mathbf{n}$ through angle φ is

$$R_{\mathbf{n}}(\varphi) = \exp\left[-i\varphi \mathbf{J}\cdot\mathbf{n}\right]. \tag{8-123a}$$

An n–fold rotation around the z–direction is denoted as $C_n \equiv C_{nz} = \exp(-i\frac{2\pi}{n}J_z)$, while a two–fold rotation around the direction $\mathbf{n}$ is

$$C_{2,\mathbf{n}} \equiv C_2^{\mathbf{n}} = \exp[-i\pi \mathbf{J}\cdot\mathbf{n}], \tag{8-123b}$$

Evidently,

$$C_{nz}^{n} = \theta,\ C_{nz}^{n+k} = \theta C_{nz}^{k}. \tag{8-124a}$$

For a two–fold rotation in any direction $\mathbf{n}$,

$$(C_2^{\mathbf{n}})^2 = \theta,\ \ C_{2x}^2 = C_{2y}^2 = C_{2z}^2 = \theta. \tag{8-124b}$$

A two–fold rotation $C_2^{\mathbf{n}}$ has four possible eigenvalues, ± 1 and $\pm i$ for s–v and d–v reps, respectively. From (8-123a) we know that a rotation around the axis $-\mathbf{n}$ through φ is equivalent to the rotation around $\mathbf{n}$ through $-\varphi$,

$$R_{-\mathbf{n}}(\omega) = R_{\mathbf{n}}(-\omega) = R_{\mathbf{n}}(\omega)^{-1}, \tag{8-125a}$$

which leads to

$$R_{-\mathbf{n}}(\pi) = R_{\mathbf{n}}(-\pi) = R_{\mathbf{n}}(3\pi) = \tilde{R}_{\mathbf{n}}(\pi) = \theta R_{\mathbf{n}}(\pi). \tag{8-125b}$$

Therefore

$$C_2^{-\mathbf{n}} = (C_2^{\mathbf{n}})^{-1} = \theta C_2^{\mathbf{n}} = \tilde{C}_2^{\mathbf{n}}. \tag{8-125c}$$

$$\tilde{C}_{2x} = (C_{2x})^{-1} = \theta C_{2x}\ . \tag{8-125d}$$

Eq. (8-125c) shows that only for s–v reps is a two–fold rotation self–inverse (i. e. the two–fold axes $\mathbf{n}$ and $-\mathbf{n}$ are the same), while for d–v reps $C_2^{\mathbf{n}} \neq C_2^{-\mathbf{n}}$, i. e. the two–fold axes $\mathbf{n}$ and $-\mathbf{n}$ are different and thus the two–fold axis $\mathbf{n}$ could be one–sided or bilateral (two–sided) .

Since J_z is an axial vector, or due to (5-90), we have

$$C_{2x}J_zC_{2x}^{-1} = -J_z, \quad C_{2z}J_zC_{2z}^{-1} = J_z. \tag{8-126a}$$

Therefore

$$C_{2x}R_z(\varphi) = R_z(-\varphi)C_{2x}. \tag{8-126b}$$

Using (8-4) and (8-126b),

$$C_2^{(\varphi)} = R_z(\varphi)C_{2x}R_z(-\varphi) = R_z(2\varphi)C_{2x}. \tag{8-126c}$$

Letting $\varphi = 90°$ we get

$$C_{2y} = C_{2z}C_{2x}.$$

A cyclic permuting of x, y, z leads to

$$C_{2x}C_{2y} = C_{2z}. \tag{8-126d}$$

Inverting (8-126d) and using (8-125d) gives $C_{2y}C_{2x} = \theta C_{2z}$. By cyclicly permuting x, y, z in the previous two equations we obtain

$$\begin{aligned} &C_{2i}C_{2j} = C_{2k},\ i,j,k = x,y,z, \text{ and cyclic permutations,} \\ &C_{2i}C_{2j} = \theta C_{2j}C_{2i},\ i \neq j = x,y,z, \\ &C_{2x}C_{2z}C_{2x}^{-1} = \theta C_{2z}. \end{aligned} \tag{8-127a}$$

Eq. (8-127a) shows that two rotations about perpendicular axes through π commute (anticommute) with one another for s–v (d–v) reps.

From (8-126c) and (8-125d) we have

$$C_2^{(\varphi)}C_2^{(0°)} = \theta R_z(2\varphi). \tag{8-127b}$$

The inversion operator $\hat{I}$ is defined as before, which changes x, y, z into $-x, -y, -z$. A distinguishing feature of the inversion $\hat{I}$ is that it commutes with any operator of point groups in both s–v and d–v reps. It has only two possible eigenvalues, $i_0 = 1, -1$.

A reflection is a product of a two–fold rotation and the inversion,

$$\sigma_i = C_{2i}\hat{I},\ i = x,y,z. \tag{8-128a}$$

Using $\hat{I}^2 = 1$ we have

$$C_{2i} = \sigma_i\hat{I}. \tag{8-128b}$$

A reflection σ has four possible eigenvalues, ± 1 and $\pm i$ for s–v and d–v reps, respectively. From (8-125c) and (8-128a) we have

$$(\sigma^{\mathbf{n}})^2 = \theta, \qquad \sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \theta, \tag{8-129a}$$

$$\sigma^{-\mathbf{n}} = (\sigma^{\mathbf{n}})^{-1} = \theta\sigma^{\mathbf{n}} = \tilde{\sigma}^{\mathbf{n}}. \tag{8-129b}$$

Therefore a reflection is self–inverse only for s–v reps, while for d–v reps, the reflection planes with the normal $\mathbf{n}$ and $-\mathbf{n}$ are different, and a reflection plane could be two–sided (bilateral) or one–sided, depending on whether there is a reflection plane perpendicular to the given reflection plane or a two–fold rotation about an axis in the plane of the reflection (see Eq. (8-130d)).

If $\mathbf{n}$ is bilateral, then $C_2^{\mathbf{n}}$ and $C_2^{-\mathbf{n}}$ ($\sigma^{\mathbf{n}}$ and $\sigma^{-\mathbf{n}}$) belong to the same class. A class consists of bilateral axes or bilateral reflections is called *non-regular class* while all other classes are called *regular classes.*

Using $C_{2i}^2 = \sigma_i^2 = \theta$ from (8-128a) we have

$$\hat{I} = \theta\sigma_i C_{2i} = \theta C_{2i}\sigma_i. \tag{8-128c}$$

From (8-127) and (8-128a) we have

$$\sigma_i\sigma_j = C_{2k},\ i,j,k = x,y,z,\ \text{and cyclic permutations}, \tag{8-130a}$$

$$[\sigma_i, C_{2i}] = 0,\ i = x,y,z, \tag{8-130b}$$

$$\begin{cases} \sigma_i\sigma_j = \theta\sigma_j\sigma_i, \\ \sigma_i C_{2j} = \theta C_{2j}\sigma_i, \quad i \neq j = x,y,z, \\ \sigma_i C_{2j} = \theta\sigma_j C_{2i}, \end{cases} \tag{8-130c}$$

$$C_{2x}\sigma_z C_{2x}^{-1} = \theta\sigma_z, \quad \sigma_x\sigma_z\sigma_x^{-1} = \theta\sigma_z. \tag{8-130d}$$

Therefore two perpendicular reflections commute (anti–commute) for s–v (d–v) reps.

Multiplying (8-127b) by the $\hat{I}^2 = 1$ we get

$$\sigma^{(\varphi)}\sigma^{(0^\circ)} = \theta R_z(2\varphi). \tag{8-131}$$

From (8-126a) we have

$$[\sigma_z, R_z(\varphi)] = 0, \tag{8-132}$$

which shows that a rotation commutes with the reflection across a plane which is perpendicular to the rotation axis,

Although the improper rotation S_{nz} is universally defined as an anti–clockwise rotation around the z axis by $2\pi/n$ followed by a reflection in the horizontal plane, its definition for the d–v reps does not strictly follow the above definition. Most of the literature follows the definition by Koster et al (page 5, 1963).

$$\sigma_z R(\varphi) = \begin{cases} S(\varphi + 2\pi), & 0 < \varphi < \pi, \\ S(\varphi), & -\pi < \varphi < 0. \end{cases} \tag{8-133a}$$

This definition is equivalent to

$$S_{nz} = \theta\sigma_z C_{nz},\ S_{nz}^{-1} = \sigma_z C_{nz}^{-1}. \tag{8-133b}$$

Using

$$S_{nz} = \theta I C_{2z} C_{nz} = \theta I C_{2n,z}^{2+n},$$

we have

$$S_{3z} = \theta\hat{I}C_{6z}^5, \quad S_{4z} = \theta\hat{I}C_{4z}^3, \quad S_{6z} = \theta\hat{I}C_{3z}^2, \quad S_{10z} = \theta\hat{I}C_{5z}^3. \tag{8-133c}$$

Therefore for both s–v and d–v cases we have

$$\hat{I}C_{3z}^{\pm} = S_{6z}^{\mp}, \quad \hat{I}C_{4z}^{\pm} = S_{4z}^{\mp}, \quad \hat{I}C_{5z}^{\pm 2} = S_{10z}^{\mp}, \quad \hat{I}C_{6z}^{\pm} = S_{3z}^{\mp}. \tag{8-133d}$$

From (8-133b) and using $\sigma_z^2 = \theta$ we also have

$$S_{2n,z}^{2k} = \theta_k C_{nz}^k\ . \tag{8-133e}$$

8.11.4. The Opechowski rule for classes

There is a rule derived by Opechowski (1940) for obtaining the classes of a double point group $G^\dagger$ from the classes of the ordinary point group G :

For a regular class i of G, the class C_i goes over to two classes, C_i and $\tilde{C}_i$ of $G^\dagger$, while for a non–regular class j of G, the class C_j goes over to the class $(C_j, \tilde{C}_j)$ of $G^\dagger$.

Proof : For regular classes $i = 1, 2, \cdots N_{\rm reg}$, we have $\tilde{C}_i = -C_i$, and thus $\chi^\nu(\tilde{C}_i) = -\chi^\nu(C_i)$. Therefore $\tilde{C}_i$ and C_i are two different classes, and the group $G^\dagger$ has $2N_{\rm reg}$ regular classes. For non–regular classes $j = 1, 2, \cdots N_{\rm non}$, according to the definition of non–regular class and Eqs. (8-125c) as well as (8-129b), $C_2^{\mathbf{n}}$ and $\tilde{C}_2^{\mathbf{n}}$ belong to the same class, or $\sigma^{\mathbf{n}}$ and $\tilde{\sigma}^{\mathbf{n}}$ belong to the same class. **QED**

We leave to readers the exercise of showing that in d-v reps the character χ_j of a non–regular class is necessarily zero.

Letting N and $N^\dagger$ be the number classes of G and $G^\dagger$, respectively, we have

$$N^\dagger = N + \tilde{N}, \quad N = N_{\rm reg} + N_{\rm non}, \ \tilde{N} = N_{\rm reg}. \tag{8-134a}$$

As we know that N is the numbers of s–v irreps of G, and we will know later that $\tilde{N} = N_{\rm reg}$ is the numbers of d–v irreps of G.

As an example, consider the group $D_n^\dagger$. The groups $D_{\rm odd}$ and C_n consist of only regular classes. They have equal number of s–v and d–v irreps ($N = \tilde{N}$), and have one–dimensional d–v irreps.

The groups $D_{\rm even}, T, O, I, T_d, T_h, O_h$ and I_h consist of both regular and non–regular classes. They have more s–v irreps than d–v irreps ($N > \tilde{N}$), and have only even–dimensional d–v irreps, which are characterized by $\chi_j = 0$ for non–regular classes.

From the above we get the classes of $D_n^\dagger$ with odd n:

$$\begin{aligned} &e, 2C_n, 2C_n^2, \cdots, C_n^{\frac{n-1}{2}}, nC_2, \\ &\tilde{e}, 2\tilde{C}_n, 2\tilde{C}_n^2, \cdots, \tilde{C}_n^{\frac{n-1}{2}}, n\tilde{C}_2, \end{aligned} \tag{8-134b}$$

where $2C_n^k = \{C_n^k, C_n^{-k}\}$, and $N = \tilde{N} = \frac{n+3}{2}$.

Notice that since there is no C_{2z} in D_n with odd n, the two–fold axes are one–sided, and nC_2 and $n\tilde{C}_2$ belong to different classes.

The classes of $D_n^\dagger$ with even n are

$$\begin{aligned} &e, 2C_n, 2C_n^2, \cdots, C_n^{\frac{n-2}{2}}, \{C_{2z}, \tilde{C}_{2z}\}, \{\tfrac{n}{2}C_2, \tfrac{n}{2}\tilde{C}_2\}, \{\tfrac{n}{2}C_2', \tfrac{n}{2}\tilde{C}_2'\}, \\ &\tilde{e}, 2\tilde{C}_n, 2\tilde{C}_n^2, \cdots, \tilde{C}_n^{\frac{n-2}{2}}, \end{aligned} \tag{8-134c}$$

with $N = \frac{n}{2} + 3, \tilde{N} = \frac{n}{2}$. Notice that since there is the element $C_{2z} = (C_{nz})^{\frac{n}{2}}$ for D_n with even n, the two–fold axes are bilateral, thus $\frac{n}{2}C_2$ and $\frac{n}{2}\tilde{C}_2$ belong to the same class, same to $\frac{n}{2}C_2'$ and $\frac{n}{2}\tilde{C}_2'$

8.11.5. The double–group method for d–v representations

Usually, the double point group $G^\dagger$ is regarded as an abstract group of order $2|G|$, and the irreps of $G^\dagger$ can be found in the usual way. Among the irreps of $G^\dagger$, some are identical to those of the point group G, which are just the single–valued reps of G, while others are not included in the irreps of G, they are the double–valued reps of G. This is called the *double–group method.*

For example, the group $D_2^\dagger$ is of order 8, and has five classes with the class operators,

$$C_1 = e\ , \quad C_2 = \tilde{e}\ , \quad C_3 = C_{2x} + \tilde{C}_{2x}\ , \quad C_4 = C_{2y} + \tilde{C}_{2y}\ , \quad C_5 = C_{2z} + \tilde{C}_{2z}\ . \tag{8-135}$$

Using the EFM of Chapter 3, and choosing $C(s) = C_{2x}$ (that is the $D_2^\dagger \supset C_{2x}^\dagger$ basis) we can find its characters as listed in Table 8.3-2 and two–dimensional irreducible matrices listed in

Table 8.11-2. The group $D_2^\dagger$ has five irreps: the four one–dimensional reps are the s–v reps of D_2, for which $D(\tilde{R}_i) = D(R_i)$, while the two–dimensional rep is the d–v irrep $E_{1/2}$ of D_2, for which $D^{E_{1/2}}(\tilde{R}_i) = -D^{E_{1/2}}(R_i)$. If we choose $C(s) = C_{2z}$, then the irrep $E_{1/2}$ will be the same as given in Table 8.11-1, where we started from.

Table 8.11-2. Double–valued rep $E_{1/2}$ of $D_2 \supset C_{2x}$. Here $D^{E_{1/2}}(\tilde{R}_i) = -D^{E_{1/2}}(R_i), i = 1, 2, 3, 4.$

e	C_{2x}	C_{2y}	C_{2z}
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$

8.12. The Representation Group and Its Applications

In this section we denote an abstract group by **G**, while the symbol $\mathcal{G}$ will denote the matrix group or operator group formed by the representations of the elements of **G**.

The double–group method, though straightforward, is not economical. The s–v irreps of point groups are all known. All we need are the d–v irreps of **G**. Can we describe a simple method for getting only d–v irreps of **G**?

Recall that in dealing with the double group $\mathbf{G}^\dagger$ in (8-121d), we regarded the elements $\pm D^{\frac{1}{2}}(\alpha_i, \beta_i, \gamma_i)$ as linearly independent, though they differ only by a sign. What if they are regarded as linearly dependent? A short answer is that the double group becomes a *representation group*, and the problem of seeking d–v reps can be greatly simplified.

8.12.1. The representation group

Definition 8.1: The representation of a group **G** in a representation space r forms a group, called the *representation group* (*rep group*) $\mathcal{G}_r$, when the linear dependence of the elements of $\mathcal{G}_r$ are taken into account.

Remark 1: The representation r may be reducible or irreducible, and may be faithful or unfaithful. The elements $R_1, R_2, \cdots$, of the rep group $\mathcal{G}_r$ are matrices or operators, which are representatives of the elements $\hat{R}_1, \hat{R}_2, \cdots$, of the group **G**.

Remark 2: A fundamental difference between a rep group and an ordinary group (that is a group in the usual sense) is that the elements of the former may be *linearly dependent* while those of the latter are always regarded as linearly independent. When all elements of a rep group are linearly independent, it reduces to the ordinary group. In this sense the ordinary group can be regarded as a special case of the rep group.

Remark 3: *The difference between a matrix group and rep group.*

If all elements of a matrix group are distinct (but may linearly dependent), and distinct elements are regarded as elements of an abstract group (thus are necessarily linearly independent), then the matrix group is identical with the abstract group. This is what a matrix group means in the conventional sense. On the other hand, if linearly dependence is taken into account, then the matrix group is a rep group. In other words, a matrix group can be regarded either as an abstract group or a rep group.

Remark 4: The rep group defined here is totally different from the representation group defined by Döring (1959) and Birman (1974), which is a group in the usual sense.

Suppose that a group **G** has N classes with N class operators $\hat{C}_i$. The representatives of $\hat{C}_i$ in the rep space r are denoted by C_i. Due to the linear dependence of the group elements of the rep group $\mathcal{G}_r$, the N class operators C_i of $\mathcal{G}_r$ are not linearly independent. Some of

the class operators may be null operators, and some may differ by only phase factors. Let $C_1(=e), C_2, \ldots, C_n$ be the linearly independent class operators of $\mathcal{G}_r$, $n \leq N$ (the equality holds only for an abstract group).

Example 1: The rep groups $\mathcal{G}_r$ of the inversion group $\mathbf{G} = (\hat{e}, \hat{I})$ in the representation spaces $r = g, u$ associated with $I = 1, -1$, are $\mathcal{G}_g = (e, e)$ and $\mathcal{G}_u = (e, -e)$, respectively. The former is unfaithful while the latter is faithful. An unfaithful rep group is used on page 5505 of Chen & Fan (1998b). Otherwise we deal only with faithful rep groups.

Example 2: The quaternion group $\mathbf{Q}$ in (1-4b) has five classes with class operators

$$C_1 = e,\ C_2 = -e,\ C_3 = (i\sigma_x) + (-i\sigma_x),\ C_4 = (i\sigma_y) + (-i\sigma_y),\ C_5 = (i\sigma_z) + (-i\sigma_z).$$

The group $\mathbf{Q} \sim \mathbf{D}_2^\dagger$ has five irreps, four one–dimensional and one two–dimensional. On the other hand, the rep group $\mathcal{Q}$ has only one linearly independent class operator, $C_1 = -C_2 = e, C_3 = C_4 = C_5 = 0$, and has only one irreducible representation, which is just the irrep $E_{1/2}$ of D_2.

Example 3: The representation of a double group $\mathbf{G}^\dagger$ in a generic spinor space forms a rep group $\mathcal{G}^\dagger$,

$$\mathcal{G}^\dagger = \{R_i, -R_i : i = 1, 2, \ldots, |G|\}\ . \tag{8-136a}$$

The linearly independent elements do not form a group. Their multiplication relations are

$$R_i R_j = \theta(i,j) R_{ij}\ ,\quad i, j = 1, 2 \cdots, |G|,\quad \theta(i,j) = \pm 1. \tag{8-136b}$$

where the $\theta(i,j)$ are said to form a *factor system* (see (2-46)). This shows that $\{R_i : i = 1, 2, \ldots, |G|\}$ forms a projective rep of the point group $\mathbf{G}$. We thus see that obtaining the d–v irreps is equivalent finding to the projective irrep of $\mathbf{G}$.

Example 4: Suppose that there is an abstract group $\mathbf{G}$,

$$\mathbf{G} = \{\widehat{R}_s : s = 1, 2, \ldots, |G|\}\ . \tag{8-137a}$$

The representation of $\mathbf{G}$ in a rep space L is

$$\mathcal{G} = \{R_s : s = 1, 2, \ldots, |G|\}\ . \tag{8-137b}$$

Suppose that among the $|G|$ elements R_s there are only $|g|$ linearly independent elements which form a set, called the *fundamental set*,

$$F = \{R_1, R_2, \ldots, R_{|g|}\}\ , \tag{8-138a}$$

and that the other elements are related to those in F by

$$R_i^{(l)} = \exp(2\pi l i/m) R_i\ ,\quad l = 0, 1, \ldots, m-1\ ,\quad |G| = m|g|\ , \tag{8-138b}$$

then

$$\mathcal{G} = \{R_i^{(l)} : i = 1, 2, \ldots, |g|,\quad l = 0, 1, \ldots, m-1\} \equiv \{R_i^{(l)} : i = 1, 2, \ldots, |g|\}_m \tag{8-138c}$$

is a *rep group*.

Notice that Example 3 is a special case of Example 4 with $m = 2$. In Chapter 10 we will deal with the rep group with $m > 2$. When $m = 1$ the rep group reduces to the ordinary group.

Definition 8.2 : The space spanned by $R_1, R_2, \ldots, R_{|g|}$ is called the *group space* L_g *of the rep group* $\mathcal{G}$.

The multiplication relations of $\mathcal{G}$ is totally specified by the $|g| \times |g|$ group table,

$$R_i R_j = \eta(i,j) R_{ij} \ , \quad i,j = 1,2\cdots, |g|, \quad |\eta(i,j)| = 1. \tag{8-138d}$$

Definition 8.3: The vector space spanned by the n linearly independent class operators $C_1, C_2, \ldots, C_n$ is referred to as the *class space* L_n *of the rep group* $\mathcal{G}$.

The n class operators form the *class algebra* of the rep group $\mathcal{G}$ with the multiplication rule

$$C_i C_j = \sum_{k=1}^{n} C_{ij}^k C_k, \quad i,j = 1,2,\ldots,n \ . \tag{8-138e}$$

Notice that now the structure constants C_{ij}^k may be negative (when $m = 2$) or imaginary (when $m > 2$).

Suppose that there is a group $\mathbf{G}_0$ of order $|G_0| = |g|$ and with elements γ_i,

$$\mathbf{G}_0 = \{\gamma_i : i = 1,2,\ldots,|g|\} \ . \tag{8-139a}$$

If $\mathbf{G}_0$ satisfies the multiplication relation

$$\gamma_i \gamma_j = \gamma_{ij}, \quad i,j = 1,2,\ldots,|g| \ , \tag{8-139b}$$

then the rep group $\mathcal{G}$ is an m–fold covering group of $\mathbf{G}_0$, and under the mapping $R_i \to \gamma_i$, the fundamental set F of $\mathcal{G}$ is a projective rep of the group $\mathbf{G}_0$.

From (8-138b), we know that an irrep λ of the rep group $\mathcal{G}$ can be specified by explicitly giving only the irreducible matrices for the $|g|$ linearly independent elements. Hence for simplicity, we shall just say that

$$D^{(\nu)}(\mathcal{G}) = \{D^{(\nu)}(R_i) : i = 1,2,\ldots,|g|\} \ , \tag{8-139c}$$

is an irrep of the rep group $\mathcal{G}$. $D^{(\nu)}(\mathcal{G})$ is clearly a projective irrep of the group $\mathbf{G}_0$ under the mapping $R_i \leftrightarrow \gamma_i$, namely, each irrep of the rep group $\mathcal{G}$ gives a projective irrep of $\mathbf{G}_0$. Therefore, the construction of projective irreps of the group $\mathbf{G}_0$ for the factor system $\eta(i,j)$ can be replaced by the construction of the vector irreps of the rep group $\mathcal{G}$, which is, as will be seen later, as easy as that for a finite group of order $|g| = |G|/m$.

On the other hand, the irreps and irreducible bases of an abstract group $\mathbf{G}$ in the rep space r are obviously identical to those of the rep group $\mathcal{G}_r$, and thus the former task can be replaced by the latter one. It is much easier to work with the rep group $\mathcal{G}_r$ than with the abstract group $\mathbf{G}$. Before proceeding with the problem of constructing irreps of a rep group, we first extend the definitions of the regular rep, the intrinsic group, and so on to rep groups.

The rep generated by the group space L_g is called the *regular rep* of $\mathcal{G}$, namely

$$\begin{aligned} R_j R_k &= \sum_{i=1}^{|g|} D_{ik}(R_j) R_i \quad j,k = 1,2,\ldots,|g| \ , \\ D_{ik}(R_j) &= \eta(j,k)\delta_{i,jk} \ . \end{aligned} \tag{8-140a}$$

Now consider the intrinsic group $\overline{\mathcal{G}}$ of a rep group $\mathcal{G}$. We first define $|g|$ operators $\overline{R}_j$ in the group space L_g by

$$\overline{R}_j R_k = R_k R_j = \eta(k,j) R_{kj} \ , \quad j,k = 1,2,\ldots,|g| \ , \tag{8-140b}$$

and define

$$\overline{R}_j^{(l)} = \exp(2\pi l i/m)\overline{R}_j \ , \quad j = 1,2,\ldots,|g| \ , \quad l = 0,1,\ldots,m-1 \ . \tag{8-140c}$$

Then

$$\overline{\mathcal{G}} = \{\overline{R}_j^{(l)} : j = 1, 2, \ldots |g| \,, \quad l = 0, 1, \ldots, m-1\} \,, \tag{8-140d}$$

forms the *intrinsic group* $\overline{\mathcal{G}}$ of the rep group $\mathcal{G}$. The regular rep $D(\overline{\mathcal{G}})$ of the intrinsic group $\overline{\mathcal{G}}$ is defined by

$$\overline{R}_j R_k = \sum_{i=1}^{|g|} D_{ik}(\overline{R}_j) R_i, \quad j, k = 1, 2, \ldots, |g| \,,$$
$$D_{ik}(\overline{R}_j) = \eta(k, j)\delta_{i,kj} \,. \tag{8-140e}$$

The new approach to the rep theory of (abstract) groups can be easily extended to the rep group (see the extensive review by Chen, Gao & Ma 1985). All the definitions of the CSCO–I, –II and –III of **G**, all the formulas and conclusions remain valid for the rep group under the substitutions

$$g(= |G|) \to |g| = |G|/m, \quad N \to n \,. \tag{8-141a}$$

For instance, Burnside's Theorem (Theorem 3.25) may be written for the rep group as

Theorem 8.1: A rep group $\mathcal{G}$ with n linearly independent class operators contains n and only n inequivalent irreps.

Theorem 8.2: The regular rep of a rep group $\mathcal{G}$ contains n inequivalent irreps, and the number of times each irrep occurs is equal to its dimension,

$$|g| = \sum_{\nu=1}^{n} h_\nu^2 \,. \tag{8-141b}$$

Therefore, the irreps and irreducible bases of the rep group can be found just as those of abstract groups. The only differences are:

1. Now the elements of the regular representation matrices of the group $\mathcal{G}$ or its intrinsic group $\overline{\mathcal{G}}$ may be imaginary, while for an abstract group, they can only be 1 or zero.

2. For a non–trivial rep group (that is, $m > 1$ instead of $m = 1$), there is no identity rep, while for an abstract group, there must be an identity rep.

3. For an abstract group **G**, the identity is never chosen as a member of the CSCO–I. If there is only one linearly independent class operator for a rep group, it must be the identity and is the CSCO of the rep group.

Example: Find the double–valued irrep of $\mathbf{D}_2$. In the spinor rep space, $\tilde{R}_i = -R_i$. From (8-135) we have

$$C_1 = e \,, \quad C_2 = -e \,, \quad C_3 = C_4 = C_5 = 0 \,.$$

This shows that the rep group $D_2^\dagger = \{\pm e, \pm C_{2x}, \pm C_{2y}, \pm C_{2z}\}$ has only one linearly independent class operator. We thus immediately know that there is only one double–valued irrep for $\mathbf{D}_2$. Now $|g| = 4$, and from (8-141b) we have $4 = 2^2$. Therefore this double–valued irrep is two–dimensional.

The CSCO–I of the rep group $\mathcal{D}_2^\dagger$ is $C = e$ and the diagonalization of C is unnecessary. The operator set $C(s)$ can be chosen as R_2. $(R_2, \bar{R}_2)$ is the CSCO–III of the rep group. By reading the group Table 8.11-1 horizontally and vertically, we can write down the regular reps of R_2 and the intrinsic element $\overline{R}_2$, respectively;

$$D(R_2) = (2\bar{1}4\bar{3}) = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad D(\bar{R}_2) = (2\bar{1}\bar{4}3) = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} . \tag{8-142}$$

We can find the common eigenvectors $\{u_{\nu mk,i} : i = 1, \ldots, 4\}$ of $D(R_2)$ and $D(\bar{R}_2)$, and adjust the phases of the eigenvectors by using (3-201). Then from (3-198) we can obtain the irrep of the rep group D_2, which is just that shown in Table 8.11-2 obtained by the double group method.

In summary, the key point of the rep group approach is that we focus our attention on the linearly independent elements of a (matrix) group instead of on the whole set of elements. The advantage of the rep group approach to this problem is now very clear. Originally, we needed to treat a group of order $m|g| = 8$, and now we only need to treat a rep group with the "effective order" $|g| = 4$. For cases with large m and large $|g|$ (for example for the single–valued reps of space groups, $m = 2, 3, 4, 6$, while for the double–valued reps of space groups, $m = 4, 6, 8, 12$, and $|g|$ can be as high as 48), a tremendous simplification results from using the rep group approach.

Ex. 8.24. Show that in d–v reps the character $\chi_j = 0$ for any non–regular class j.

Ex. 8.25. Show that the number of linearly independent class operators of a rep group $\mathcal{G}^\dagger$ is equal to half the number of the regular classes of $G^\dagger$, $n = N_{\text{reg}}$.

Ex. 8.26. Show that a group with non–regular classes has no odd–dimensional irreps. *Hints*: 1. In a d–v reps the character of non–regular class is necessarily zero. 2. The possible values of C_{2x} or σ_x are $\pm 1, \pm i$.

Ex. 8.27. Show that all the multi–dimensional irreps of any point group are even–dimensional.

Ex. 8.28. Find the CSCO–I and characters of the rep group $\mathcal{D}_3^\dagger$. The group table is given below.

Table 8.12-1. Group table of $D_3^\dagger$.

e	C_3	C_3^2	C_{21}	C_{22}	C_{23}
1	2	3	4	5	6
2	−3	1	−6	−4	−5
3	1	−2	5	−6	−4
4	−5	−6	−1	2	3
5	−6	−4	3	−1	2
6	−4	−5	2	3	−1

Ex. 8.29. Find the double–valued irreps of $\mathbf{D}_3$ in the $\mathbf{D}_3 \supset (\mathbf{e}, C_{21})$ basis.

8.12.2. Characters of d–v irreps of point groups

For a double group $\mathbf{G}^\dagger$ the frequency for the irrep Γ to appear in the subduced rep $j^\pi \downarrow \mathbf{G}^\dagger$ is given by (compare with (8-71b))

$$\tau_\lambda = \frac{1}{|2G|} \sum_{a=1}^{2|G|} \chi^{(\lambda)}(R_a)^* \chi^{(j\ell)}(R_a), \quad \pi = (-1)^\ell, \tag{8-143a}$$

where $\chi^{(j\ell)}(R_a)$ is the character of the element R_a in the subduced representation $j^\pi \downarrow \mathbf{G}$. Since

$$\chi^{(\lambda)}(R_a)^* \chi^{(j\ell)}(R_a) = \chi^{(\lambda)}(R_a + 2\pi)^* \chi^{(j\ell)}(R_a + 2\pi),$$

Eq. (8-143a) is reduced to

$$\tau_\lambda = \frac{1}{|G|} \sum_{a=1}^{|G|} \chi^{(\lambda)}(R_a)^* \chi^{(j\ell)}(R_a). \tag{8-143b}$$

In other words, in practice we only need the characters of the elements $R(\varphi), 0 \le \varphi \le 2\pi$, and not those $\bar{R}(\varphi) = R(\varphi + 2\pi)$. In most textbooks which deal with double–valued reps, the

characters for both the elements R and $\tilde{R}$ are listed. This is a waste of space, and unnecessarily complicated. The character tables for the d–v reps of point groups are given in Table 8.3-2 to Table 8.3-9, where the characters of the elements $\tilde{R}$ in the regular classes are not listed.

Actually we can go one step further by claiming that we only need the characters of any $|G|$ linearly independent elements, say $R'_1, R'_2, \cdots, R'_{|G|}$, where R'_i is either R_i or $-R_i$, since we have

$$\tau_\lambda = \frac{1}{|G|}\sum_{a=1}^{|G|}\chi^{(\lambda)}(R'_a)^*\chi^{(j\ell)}(R'_a). \tag{8-143c}$$

We will meet such a choice for the linearly independent elements of the group C_{nh} in Sec. 8.12.3.

8.12.3. Algebraic solutions for cyclic groups C_n, S_{2n} and C_{nh}

The discussions in Sec. 8.12.1 suggest a unified method for finding s–v and d–v irreps of a point group G. Let us introduce the representation group

$$\mathcal{G}(\theta) = \{R_a, \theta R_a : a = 1, 2, \cdots, |G|\} \tag{8-144}$$

which depends on the parameter $\theta = \pm 1$. By replacing the elements $\tilde{R}_a$ by θR_a, the group table becomes a function of θ. We can use the EFM to find the algebraic expressions for the projection operators $\mathcal{P}_\mu^{(\lambda)\bar{\mu}}$ of the rep group $\mathcal{G}(\theta)$ as a function of θ. The eigenvalues $\lambda, \mu, \bar{\mu}$ are also functions of θ. The solutions associated with $\theta = 1$ and -1 correspond to the s–v and d–v cases, respectively. The algebraic solutions for dihedral groups and other point groups can actually be calculated in this way. It is only for pedagogical reasons that the s–v and d–v cases are treated separately. The algebraic solutions for all point groups have been found in this way (Fan, Chen & Draayer 1999 and references therein). In this section we will find the algebraic solutions for all cyclic point groups for both s–v and d–v cases.

The algebraic solution for the group C_n is already known, with the character and SAF's obtained from (8-48b) and given explicitly as

$$\chi^{(\mu)}(C_{nz}^k) = \exp(-\tfrac{2k\mu\pi}{n}i); \qquad \psi^\mu = |jm\rangle, \quad m \doteq \mu\,. \tag{8-145}$$

The group S_{2n} with even n

It is well known that the group S_{2n} is isomorphic to C_{2n}. However there are many ways of realizing the isomorphism between the elements of the two groups. One possible isomorphic mapping is: $(S_{2n,z}^{k'})^j \longleftrightarrow (C_{2n,z}^k)^j$ for $j = 0, 1, \cdots, 2n-1$, with any given odd k and k'. Choosing an appropriate mapping is the key in obtaining the SAF's of S_{2n} from those of C_{2n} in a straightforward manner (more precisely, the SAF's of S_{2n} for even parity are required to be the same as the SAF's of C_{2n}).

The improper rotation is defined in (8-133b). To obtain unified algebraic solutions for s–v and d–v reps, the most natural definition is

$$S'_{nz} \equiv \sigma_z C_{nz} = \theta S_{nz}\,. \tag{8-146a}$$

In the following derivation we use S'_{nz} for simplicity, but will switch back to the usual definition (8-133b) in the final expressions, so that no confusion will arise. Firstly we transform the expression for $S_{2n,z}^{'k}$ in the following way:

$$(S'_{2n,z})^k = C_{2n,z}^k(\sigma_z)^k = C_{2n,z}^k(\hat{I}C_{2,z})^k = \hat{I}^k C_{2n,z}^{(n+1)k}\,. \tag{8-146b}$$

Noting that $C_{2n,z}^{(n+1)k}$ are elements of C_{2n}, we obtain the characters of $S_{2n} \sim C_{2n}$ from those of C_{2n} with the following replacements

$$C_{2n,z}^{(n+1)k} \to S_{2n,z}^{'k}\,. \tag{8-146c}$$

It is seen that instead of the naive mapping $S'_{2n,z} \to C_{2n,z}$, we choose the mapping as $S'_{2n,z} \to C^{n+1}_{2n,z}$. However, the latter mapping only ensures the isomorphism $S_{2n} \sim C_{2n}$ when n is even. When n is odd $C^{(n+1)k}_{2n,z} = C^{(n+1)k/2}_{nz}$, and we only have the homomorphic mapping $S_{2n} \to C_n$.

To ensure that the isomorphic mapping $S'^k_{2n,z} \to C^{(n+1)k}_{2n,z}$ imposed in (8-146c) can be used, we rewrite the projection operators of C_{2n} given in (8-37a) in the following way,

$$P^{\epsilon_\mu}(C_{2n}) = \frac{1}{2n}\sum_{k=0}^{2n-1}(\epsilon^*_\mu)^{(n+1)k}C^{(n+1)k}_{2n,z} \ , \tag{8-147a}$$

with $\epsilon_\mu = \exp(-\frac{\mu\pi}{n}i)$. Using (8-146c) we then find the projection operators of S_{2n} to be

$$P^{\epsilon_\mu}(S_{2n}) = \frac{1}{2n}\sum_{k=0}^{2n-1}(\epsilon^*_\mu)^{(n+1)k}S'^k_{2n,z} \ . \tag{8-147b}$$

The irreps of S_{2n} are still labelled by the quantum number μ. The characters of S_{2n} in the irrep μ can be obtained from (8-147b) and (8-146a).

$$\chi^{(\mu)}(S^k_{2n,z}) = (\theta_\mu)^k(\epsilon_\mu)^{(n+1)k} = (\theta_\mu\omega^{(n+1)\mu})^k, \tag{8-148a}$$
$$\omega = \exp\big(-\tfrac{\pi}{n}i\big) = \epsilon_1, \quad \theta_\mu = (-1)^{2\mu}.$$

Due to (8-133e) a formula for the character of C^k_{nz} is unnecessary.

The CSCO of S_{2n} and its eigenvalue are

$$C = S_{2n,z}, \quad \lambda_\mu = \theta_\mu\omega^{(n+1)\mu}, \quad \mu = 0, \pm\tfrac{1}{2}, \pm 1, \pm(n-\tfrac{1}{2}), n \ . \tag{8-148b}$$

The CSCO is useful for checking whether a vector is an irreducible basis vector of S_{2n}.

With the operator $S_{2n,z}$ the projection operators of S_{2n} in (8-147b) can be re-written as

$$P^{\mu}(S_{2n}) = \frac{1}{2n}\sum_{k=0}^{2n-1}(\lambda^*_\mu)^k S^k_{2n,z} \ . \tag{8-147c}$$

The SAF's of C_n do not depend on the parity $(-1)^\ell$ of the state, while those of improper cyclic groups do. We use $|\ell jm\rangle$ to denote a many-particle state with the parity $(-1)^\ell = \pm 1$, total angular momentum j and its projection m. For a single-particle state, ℓ is identified with the orbital angular momentum l, and in the s–v representations we have $j = l = \ell$.

Applying the projection operator of S_{2n} in (8-147b) to $|\ell jm\rangle$ and using (8-146b) we have

$$\begin{aligned} P^{\epsilon_\mu}(S_{2n})|\ell jm\rangle &= \tfrac{1}{2n}\sum_{k=0}^{2n-1}(\epsilon^*_\mu\epsilon_m)^{(n+1)k}(-)^{\ell k}|\ell jm\rangle \\ &= \delta_{\mu',m(\mathrm{mod}\,2n)}|\ell jm\rangle, \ \mu' = \mu - \tfrac{1-(-1)^\ell}{2}n \ , \end{aligned} \tag{8-149a}$$

where in obtaining the last equation we use the relations (noting that n is even)

$$\begin{aligned} \tfrac{1}{2n}\sum_{k=0}^{2n-1}(\epsilon^*_\mu\epsilon_m)^{(n+1)k}(-1)^k &= \tfrac{1}{2n}\sum_{k=0}^{2n-1}(-\epsilon^*_\mu\epsilon_m)^{(n+1)k} \\ = \tfrac{1}{2n}\sum_{k=0}^{2n-1}(\epsilon^*_{\mu-n}\epsilon_m)^{(n+1)k} &= \delta_{\mu-n,m(\mathrm{mod}\,2n)} \ . \end{aligned}$$

From (8-149a) we obtain the SAF's of S_{2n} for even n:

$$\psi^{\mu} = |\ell j m\rangle, \quad m = \mu - \tfrac{1-(-1)^{\ell}}{2} n \ (\text{mod } 2n) \ . \tag{8-149b}$$

As a check, by applying the CSCO $S_{2n,z}$ of S_{2n} to $|\ell j m\rangle$ and using (8-146b), we will find that $|\ell j m\rangle$ is an eigenvector of $S_{2n,z}$ with eigenvalues $\exp\big(-(\mu - \frac{1-(-1)^{\ell}}{2} n)\frac{(n+1)\pi}{n} i\big), \mu = m \ (\text{mod } n)$. Therefore $|\ell j m\rangle$ belongs to the irrep $\mu - \frac{1-(-1)^{\ell}}{2} n, \mu = m \ (\text{mod } n)$.

It is seen that the SAF's of S_{2n} for even parity are identical with the SAF's of C_{2n}. This simple relationship is obtained only for the mapping (8-146c), $C_{2n,z}^{(n+1)k} \leftrightarrow S_{2n,z}^{\prime k}$.

The group C_{nh} with odd n

Let us first introduce

$$\mathcal{S}_{nz}^{(k)} \equiv \sigma_z C_{nz}^{k} \ . \tag{8-150a}$$

Notice the difference between $\mathcal{S}_{nz}^{(k)} = \sigma_z C_{nz}^{k}$ and $S_{nz}^{\prime k} = (\sigma_z C_{nz})^k$. The relationship between the two is

$$\begin{aligned} &\mathcal{S}_{nz} \equiv \mathcal{S}_{nz}^{(1)} = \theta S_{nz}, \\ &\mathcal{S}_{nz}^{(2k+1)} = \theta^k S_{nz}^{\prime 2k+1} = \theta^{k+1} S_{nz}^{2k+1} \ . \end{aligned} \tag{8-150b}$$

For example, for C_{3h} we have

$$\mathcal{S}_{3z}^{(0)} = \sigma_z \ , \ \mathcal{S}_{3z}^{(1)} = \sigma_z C_{3z} = \theta S_{3z} \ , \ \mathcal{S}_{3z}^{(2)} = \theta \sigma_z C_{3z}^{-1} = \theta S_{3z}^{-1} \ . \tag{8-150c}$$

The group C_{nh} can now be expressed as

$$C_{nh} = \{C_{nz}^{k}, \mathcal{S}_{nz}^{(k)} : k = 0, 1, \cdots, n-1\}. \tag{8-150d}$$

To implement the isomorphism between C_{nh} and C_{2n} we transform the expressions of $\mathcal{S}_{nz}^{(k)}$ in the following way:

$$\mathcal{S}_{nz}^{(k)} = \hat{I} C_{2z} C_{nz}^{k} = \hat{I} C_{2n,z}^{2k+n} \ . \tag{8-151a}$$

Therefore the group C_{nh} is isomorphic to the group C_{2n} under the following mapping

$$\mathcal{S}_{nz}^{(k)} \longleftrightarrow C_{2n,z}^{2k+n} \ . \tag{8-151b}$$

The projection operators for C_{2n} can be written as

$$P^{\epsilon_\mu}(C_{2n}) = \tfrac{1}{2n} \sum_{k=0}^{n-1} \left[(\epsilon_\mu^*)^{2k} C_{2n,z}^{2k} + (\epsilon_\mu^*)^{2k+n} C_{2n,z}^{2k+n}\right] \ ,$$

with $\epsilon_\mu = \exp(-\frac{\pi\mu}{n} i)$ still. Using the mapping in (8-151b) we obtain the projection operator of C_{nh} with odd n,

$$P^{\epsilon_\mu}(C_{nh}) = \tfrac{1}{2n} \sum_{k=0}^{n-1} \left[(\epsilon_\mu^*)^{2k} C_{nz}^{k} + (\epsilon_\mu^*)^{2k+n} \mathcal{S}_{nz}^{(k)}\right] \ . \tag{8-152a}$$

Applying the projection operator (8-152a) of C_{nh} to $|\ell j m\rangle$ and using (8-151a) and (3-221b) we obtain

$$\begin{aligned} P^{\epsilon_\mu}(C_{nh})|\ell j m\rangle &= \tfrac{1}{2n} \sum_{k=0}^{n-1} \left[(\epsilon_\mu^* \epsilon_m)^{2k} + (-1)^{\ell} (\epsilon_\mu^* \epsilon_m)^{2k+n}\right] |\ell j m\rangle \\ &= \delta_{\mu', m(\text{mod } 2n)} |\ell j m\rangle \ \ \mu' = \mu - \tfrac{1-(-1)^{\ell}}{2} n \ . \end{aligned} \tag{8-152b}$$

It is seen that the SAF's of C_{nh} with odd n have the same expressions as given in (8-149b). From the definition (8-133b) we have

$$S_{nz}^{n} = \theta^{\frac{n-1}{2}}\sigma_z = \begin{cases} \theta\sigma_z, & n = 3 \text{ (mod } 4) \\ \sigma_z, & n = 5 \text{ (mod } 4) \end{cases}, \tag{8-153a}$$

$$S_{nz}^{2n} = \theta\ . \tag{8-153b}$$

Therefore the double group $C_{nh}^{\dagger}$ n = odd is the group generated from S_{nz},

$$C_{nh}^{\dagger} = \{S_{nz}^{k} : k = 1, 2, \cdots, 4n\}. \tag{8-153c}$$

In double–valued reps, among the $4n$ elements of $C_{nh}^{\dagger}$ there are only $2n$ linearly independent elements. According to Sc. 8.12.2 we only need focus on the linearly independent elements, which can be chosen freely. For the group C_{nh}, we choose the $2n$ linearly independent elements as

$$\{S_{nz}^{k} : k = 1, 2, \cdots, 2n\}.$$

For example the chosen linearly independent elements of the group C_{3h} and C_{5h} are as follows

S_{3z}	S_{3z}^{2}	S_{3z}^{3}	S_{3z}^{4}	S_{3z}^{5}	S_{3z}^{6}
S_{3z}	C_{3z}^{-1}	$\theta\sigma_z$	θC_{3z}	θS_{3z}^{-1}	θ

S_{5z}	S_{5z}^{2}	S_{5z}^{3}	S_{5z}^{4}	S_{5z}^{5}	S_{5z}^{6}	S_{5z}^{7}	S_{5z}^{8}	S_{5z}^{9}	S_{5z}^{10}
S_{5z}	θC_{5z}^{2}	S_{5z}^{3}	θC_{5z}^{-1}	σ_z	C_{5z}	θS_{5z}^{-3}	C_{5z}^{-2}	θS_{5z}^{-1}	θ

The irreps of C_{nh} are again labelled by μ. The character of C_{nh} in the irrep μ is obtained from (8-150b) and (8-152a),,

$$\chi^{(\mu)}(S_{nz}^{k}) = \left(\theta_\mu \omega^{(n+2)\mu}\right)^{k}, \quad \omega = \exp\left(-\tfrac{\pi}{n}i\right). \tag{8-154a}$$

The CSCO of C_{nh} is,

$$C = S_{nz} = \hat{\theta}\hat{I}C_{2n,z}^{n+2}, \tag{8-154b}$$

which has $4 \times n$ distinct eigenvalues

$$\lambda_\mu = \theta_\mu \omega^{(n+2)\mu}. \tag{8-154c}$$

The projection operators for C_{nh} in (8-152a) can be re-written in a simpler form as

$$P^{\mu}(C_{nh}) = \tfrac{1}{2n}\sum_{k=0}^{2n-1}(\lambda_\mu^{*})^{k} S_{nz}^{k}, \tag{8-154d}$$

which is to be compared with the projection operator (8-147c) of S_{2n}. It is also interesting to compare the eigenvalues of the CSCO's of S_{2n} and C_{nh}, (8-148b) and (8-154c), and notice that the power indices of ω, $(n+1)$ and $(n+2)$, are odd in both cases (n = even for S_{2n} and n = odd C_{nh}.)

The striking similarities between the S_{2n} with even n and C_{nh} with odd n suggest they could be regarded as cases of the one kind of groups, say X_n, with n = even and odd, respectively.

Equations (8-145), (8-148a) and (8-154a) give the characters of all cyclic point groups, which can reproduce all the relevant tables in Altmann & Herzig (1994).

Applying P^{μ} in (8-37) to the product state $|\mu_1\mu_2\rangle$ we obtain the CG series and CG coefficients of C_n:

$$\psi^{\mu} = |\mu_1\mu_2\rangle, \qquad \mu_1 + \mu_2 = \mu \ (\text{mod } n).$$

8.12.4. Algebraic solutions for dihedral groups D_n in d-v reps

In this section we only present the results for the d-v reps of the dihedral groups. The results for the d-v case are very similar to those for the s-v case, with the difference being that in the d-v reps the quantum numbers μ of C_n are all half-integer, while the eigenvalue ν of C_{2x} is imaginary, $\nu = \pm i$.

There is no one-dimensional d-v irreps for D_n with even n, while for D_n with odd n the one-dimensional projection operators is the same as (8-37c) but with different eigenvalues for ρ and ν,

$$\mathcal{P}^{A_{\rho\nu}} = P^{\rho}\wp^{\nu} = P^{\rho}(1 + \nu^* C_{2x}), \quad \rho = -1, \ \nu = \pm i. \tag{8-155a}$$

The $D_n \supset \mathcal{C}_{2x}$ and $\bar{D}_n \supset \bar{C}_n$ projection operator (compare with (8-39)),

$$\begin{cases} \mathcal{P}^{(E_{|\mu|})}_{\nu,\mu} = \wp^{\nu} P^{\mu} = [P^{\mu} + \nu^* P^{-\mu} C_{2x}], \\ \mathcal{P}^{(E_{|\mu|})}_{-\nu,\mu} = \frac{1}{i}\wp^{-\nu} P^{\mu} = \frac{1}{i}[P^{\mu} - \nu^* P^{-\mu} C_{2x}], \end{cases} \quad \nu = i, \tag{8-155b}$$

with the range of $|\mu|$ as

$$|\mu| = \tfrac{1}{2}, \tfrac{3}{2}, \cdots \begin{cases} \frac{n-1}{2}, & n = \text{even}, \\ \frac{n}{2} - 1, & n = \text{odd}. \end{cases} \tag{8-155c}$$

The $D_n \supset C_n$ projection operators (compare with (8-41b))

$$\begin{cases} \mathcal{P}^{(E_{|\mu|})}_{\mu,\mu} = P^{\mu}, \\ \mathcal{P}^{(E_{|\mu|})}_{-\mu,\mu} = -iP^{-\mu} C_{2x}. \end{cases} \tag{8-156}$$

The $D_n \supset \mathcal{C}_{2x}$ projection operators are the same as (8-43) with the convention $\text{sign}(\nu) = \pm 1$ for $\nu = \pm i$.

The $D_n \supset C_n$ irreducible matrices are (compare with (8-45b))

$$D^{E_{\mu}}(C^k_{nz}) = \begin{pmatrix} e^{-\varphi_k i}, & 0 \\ 0, & e^{\varphi_k i} \end{pmatrix}, D^{E_{\mu}}(C_{2k}) = i \begin{pmatrix} 0, & e^{-\varphi_k i} \\ e^{\varphi_k i}, & 0 \end{pmatrix}, \tag{8-157a}$$

with $\varphi_k = \frac{2k\mu\pi}{n}$. The irreducible matrices in the $D_n \supset \mathcal{C}_{2x}$ basis are (compare with (8-46b))

$$\mathbf{D}^{E_{\mu}}(C^k_{nz}) = \begin{pmatrix} \cos\varphi_k, & -\sin\varphi_k \\ \sin\varphi_k, & \cos\varphi_k \end{pmatrix}, \ \mathbf{D}^{E_{\mu}}(C_{2k}) = i \begin{pmatrix} \cos\varphi_k, & \sin\varphi_k \\ \sin\varphi_k, & -\cos\varphi_k \end{pmatrix}. \tag{8-157b}$$

From (8-157b) we can get the numerical results shown in Table 8.5-1 and Table 8.5-2.

The algebraic expression for the characters of D_n in the d-v rep is the same as (8-47).

The SAF's in the d-v case are also very similar to the s-v case.

One-dimensional SAF's

Similar to (8-49a) we have

$$\psi^{A_{-1,\nu}} = |jm\rangle + (-)^j \nu |j - m\rangle, \quad \nu = \pm i, m = \tfrac{n}{2} \ (\text{mod } n). \tag{8-158a}$$

Two-dimensional SAF's

1). $D_n \supset C_n$ basis (compare with (8-49c)):

$$\begin{cases} \psi_{\mu}^{E_\mu} = |jm\rangle, \\ \psi_{-\mu}^{E_\mu} = (-)^{j+\frac{1}{2}}|j-m\rangle, \end{cases} \quad \mu > 0,\ m = \mu \pmod{n}. \tag{8-158b}$$

2). $D_n \supset \mathcal{C}_{2x}$ basis (compare with (8-48d)):

$$\begin{cases} \psi_{i}^{E_\mu} = |jm\rangle + i(-)^j|j-m\rangle, \\ \psi_{-i}^{E_\mu} = \frac{1}{i}\left[|jm\rangle - i(-)^j|j-m\rangle\right], \end{cases} \quad m = \mu \pmod{n}. \tag{8-158c}$$

The d–v SAF's of improper dihedral groups can be obtained from those of D_n by using the same rules specified in Eq. (8-51) and (8.52).

The d–v irreducible matrices for improper dihedral groups are listed in Table 8.5-3 to Table 8.5-5. In comparing our results with others one should firstly notice the difference in the choice of positive directions of two–fold axes or reflections, and secondly the following relations derived from (8-125c),

$$D^{(\lambda)}(C_2^{-\mathbf{n}}) = \theta D^{(\lambda)}(C_2^{\mathbf{n}}), \quad D^{(\lambda)}(\sigma^{-\mathbf{n}}) = \theta D^{(\lambda)}(\sigma^{\mathbf{n}}). \tag{8-159}$$

Ex. 8.30. From (8-47) and (8-46) construct the character table and irreducible matrices for d–v reps of the group D_6, and compare them with Table 8.3-6 and Table 8.5-2.

8.13. The Time Reversal Symmetry

8.13.1. The time reversal operator

The transformation $t \to -t$ is called time reversal transformation (Sachs 1987). The symmetry is respected by all known forces except in isolated instances such as natural "K-meson" decay (Commins 1983). We denote the time reversal operator by $\hat{T}$. Under time reversal the spatial position, momentum and angular momentum transform as

$$\hat{T}\mathbf{r}\hat{T}^{-1} = \mathbf{r}, \quad \hat{T}\mathbf{p}\hat{T}^{-1} = -\mathbf{p}, \quad \hat{T}\mathbf{J}\hat{T}^{-1} = -\mathbf{J}. \tag{8-160a}$$

From (8-126a) we know that the operator J_z anti–commutes with a rotation about the y–axis through π

$$C_{2y}J_z = -J_zC_{2y}. \tag{8-160b}$$

The operator $\hat{T}$ commutes with $\mathbf{J}^2$. Using (8-160) it can be shown that the operator $\hat{T}C_{2y}$ commutes with J_z. Thus we have

$$[\hat{T}C_{2y}, \mathbf{J}^2] = 0, \quad [\hat{T}C_{2y}, J_z] = 0\ .$$

Therefore $TC_{2y}, \mathbf{J}^2$ and J_z can have simultaneous eigenvectors $|jm\rangle$. By suitably choosing the phases, the eigenvalues of $\hat{T}C_{2y}$ may be set to unity,

$$\hat{T}C_{2y}|jm\rangle = |jm\rangle\ . \tag{8-161a}$$

From Rose (1957)

$$C_{2y}|jm\rangle = (-1)^{j-m}|j-m\rangle\ .$$

Combining the last two equations we find the effect of time reversal on the eigenvectors to be,

$$\hat{T}|jm\rangle = (-1)^{j+m}|j-m\rangle. \tag{8-161b}$$

Acting with $\hat{T}$ on both sides of (8-161b) one sees that

$$\hat{T}^2 = (-1)^{2j} \equiv (-1)^N\ , \tag{8-162}$$

where N is the number of fermions.

It can be shown (Bohr 1969) that the operator $\hat{T}$ is a product of the unitary operator $i\sigma_y$ and an operator K, which implies taking complex conjugation of all c numbers,

$$\hat{T} = i\sigma_y K. \tag{8-163a}$$

For an N–particle system,

$$\hat{T} = (i)^N \sigma_y^{(1)} \cdots \sigma_y^{(N)} K. \tag{8-163b}$$

The time–reversal operator $\hat{T}$ is anti–linear and anti–unitary (Wigner 1959, chapter 26), that is

$$\hat{T}\Big(\sum_k c_k \psi_k\Big) = \sum_k (c_k)^* \hat{T}\psi_k \ , \tag{8-163c}$$

$$\langle \hat{T}\varphi | \hat{T}\psi \rangle = \langle \varphi | \psi \rangle^* = \langle \psi | \varphi \rangle. \tag{8-163d}$$

Due to the anti–linearity, it is not possible to associate a quantum number with the operator $\hat{T}$. Suppose that ψ_k is an eigenstate of $\hat{T}$, the eigenvalue depends on the phase of ψ_k. Thus if

$$\hat{T}\psi_k = \exp(i\varphi_k)\psi_k,$$

by letting $\psi_k \to \psi_k' = \exp(i\varphi_k/2)\psi_k$, we get an eigenstate with eigenvalue unity,

$$\hat{T}\psi_k' = \psi_k' \ . \tag{8-164}$$

From (8-162) we know that for odd N (double–valued representation) there are no eigenstates of $\hat{T}$, since according to (8-164) any eigenstate of $\hat{T}$ has $\hat{T}^2 = +1$.

8.13.2. The time reversal group

The set of operators $\{(\hat{T})^j : j = 0, \cdots, 3\}$ form a group, which we call the time–reversal group $\mathbf{T}$. Since $\hat{T}^2 = \hat{e}(-\hat{e})$ for s–v (d–v) representations, the group $\mathbf{T}$ is isomorphic to the double group $C_2^\dagger$.

Suppose a system has spatial symmetry G and time reversal symmetry. Since $\mathbf{T}$ and G commute, the total symmetry group of the system is a direct product G and $\mathbf{T}$, called the *magnetic point group* $\mathbf{M}$ (Wigner 1959, Bradley 1972), which can be expressed in terms of left cosets with respect to G,

$$\mathbf{M} = G \times \mathbf{T} = G + G\hat{T} \ .$$

Therefore the group $\mathbf{T}$ is the simplest magnetic point group. The representation of the magnetic group $\mathbf{M}$ is called the *co–representation* (Bradley 1972).

Instead of discussing a general co–representation, in the following we only discuss the representation of the group $\mathbf{T}$.

Although the group $\mathbf{T}$ is isomorphic to $C_2^\dagger$, the representation theory of finite groups cannot be applied to $\mathbf{T}$, because it contains both the linear and unitary operators $\pm e$ as well as anti-linear and anti-unitary operation $\pm\hat{T}$. Nevertheless, the concept of the representation, the irreducible space (the minimum invariant subspace under $\hat{T}$) and the irreducible representation remain valid.

The representation of the operator $\hat{T} = i\sigma_y K$ in the basis $\{\psi_j\}$ is denoted by $D(\hat{T})$,

$$\hat{T}\psi_j = \sum_k D(\hat{T})_{kj}\psi_k.$$

Suppose that we change basis from $|\psi_j\rangle$ to a new one $|\psi'_j\rangle$ through a linear transformation $B = (b_{ik})$:

$$\psi'_j = \sum_k b_{jk}\psi_k \ . \tag{8-165a}$$

Applying $\hat{T}$ to Eq. (8-165a) one obtains

$$\begin{aligned}\hat{T}\psi'_j &= \sum_k (b_{jk})^* \hat{T}\psi_k = \sum_{k\ell} (b_{jk})^* D(\hat{T})_{\ell k}\psi_\ell \\ &= \sum_{k\ell i} (b_{jk})^* D(\hat{T})_{\ell k}(B^{-1})_{\ell i}\psi'_i = \sum_i D'(\hat{T})_{ij}\psi'_i.\end{aligned} \tag{8-165b}$$

Therefore the new and old representations of $\hat{T}$ are related by

$$D'(\hat{T}) = \tilde{B}^{-1} D(\hat{T}) \tilde{B}^*, \tag{8-166a}$$

which is to be compared to the representation transformation (2-31a) for the spatial (linear and unitary) operator R. For a unitary transformation $B^{-1} = B^\dagger$, Eq. (8-166a) becomes

$$D'(\hat{T}) = B^* D(\hat{T}) B^{-1}. \tag{8-166b}$$

Two representations of $\mathbf{T}$ are said to be equivalent if they are related to each other as shown in (8-166a) or (8-166b), otherwise they are inequivalent. A representation $D(\hat{T})$ is said to be irreducible if it cannot be brought to a diagonalized form through the transformation (8-166a,b).

Equations (8-166a,b) show that the traces of two equivalent representation matrices of $\hat{T}$ are no longer equal. Consequently the concept of character, which is vital for the group representation theory, is invalid, and all the character theory based theorems commonly used for the usual groups break down.

For example in the s–v reps the group $\mathbf{T}$ has only one inequivalent irrep, the identity representation, with the projection operators

$$P^{(\pm 1)} = (\pm 1)^{1/2}\left(\hat{e} \pm \hat{T}\right).$$

In the d–v reps, $\hat{T}^2 = -\hat{e}$. The projection operators $P^{(\pm)} = \hat{e} \pm \hat{T}$ carry a two–dimensional irrep of $\mathbf{T}$ with the representation matrix

$$D(\hat{T}) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{8-166c}$$

which obey $D(\hat{T})^2 = -\mathbf{I}$. Consequently, *in the d–v representation space the group* $\mathbf{T}$ *has only one two–dimensional inequivalent irreducible representation.*

Equation (5-156c) can be obtained from the general expression of a co–representation in (7.3.17) in Bradley (1972) by setting $A = B = \hat{T}$ and using $\hat{T}^2 = -e$. According to (7.3.17) in Bradley (1972), the co–representation of $\hat{T}$ in a s–v rep space is

$$D(\hat{T}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} . \tag{8-166d}$$

We leave it as an exercise to the readers to show that the representation (8-166d) is a reducible representation of $\mathbf{T}$.

8.13.3. The three types of irreps

The irreps of all groups are classified into three types, the type a (potential real), type b (pseudo real) and type c (complex) (Sec. 3.12). The types of irreps of all point groups are listed in Tables 8.3-1 to 8.3-9. The following rules are helpful for memorizing the types of all irreps of point groups:

1. An irrep with complex characters $\chi^{(\lambda)}$ belongs to the type c.

2. An irrep with real characters is either of type a for all s–v reps of any point group and for the d–v irrep $\frac{n}{2}$ of the cyclic group C_n with odd n, or is of type b for all d–v irreps of any point group.

It is observed from Tables 8.3-1 to 8.3-9 that s–v irreps are either of type a or c, while d–v irreps can be of any type. Therefore irreps of type b are necessarily double–valued. Except for the tetrahedral group T, all s–v irreps of non–Abelian point groups are of type a and multi–dimensional d–v irreps are of type b. The group T has complex s–v irreps $A_{\pm 1}$ and complex two-dimensional d–v irreps $E_{\pm 3/2}$.

8.13.4. The degeneracy due to time reversal symmetry

As we know, any symmetry is related to degeneracy. Kramers' theorem states that the degeneracy due to time reversal symmetry, for a system with odd N, is at least equal to two. Wigner (1932) extended the theorem to the general case when a system also has a spatial symmetry group G. A simple approach to the problem is given below.

Consider a system with N fermions which has spatial symmetry G and the time reversal symmetry. Suppose that $\psi_\rho^{(\lambda)E_\lambda} \equiv \psi_\rho^{(\lambda)E}$ are eigenfunctions of the Hamiltonian H, which carry the irreducible representations λ and ρ of the group G and its subgroup $G(s)$, respectively. The states $\psi_\rho^{(\lambda)E}$ obey the eigenvalue equations

$$\begin{pmatrix} C \\ C(s) \\ H \end{pmatrix} \psi_\rho^{(\lambda)E} = \begin{pmatrix} \lambda \\ \rho \\ E \end{pmatrix} \psi_\rho^{(\lambda)E}, \tag{8-167a}$$

where $(C, C(s))$ is the CSCO–II of G.

It is assumed that there is no accidental degeneracy, which means that the operator set $(C, C(s), H)$ is a complete set and that corresponding to each set of eigenvalues (λ, ρ, E) there is a unique eigenvector $\psi_\rho^{(\lambda)E}$.

Applying $\hat{T}$ to both sides of (8-167a), using $[H, \hat{T}] = 0$ and the commutability of time reversal with the spatial symmetry elements, we get

$$\begin{pmatrix} C \\ C(s) \\ H \end{pmatrix} \hat{T}\psi_\rho^{(\lambda)E} = \begin{pmatrix} \lambda^* \\ \rho^* \\ E \end{pmatrix} \hat{T}\psi_\rho^{(\lambda)E}, \tag{8-167b}$$

This shows that $\hat{T}\psi_\rho^{(\lambda)E}$ is an eigenvector of H with the same eigenenergy E and is the $G \supset G(s)$ irreducible basis vector $\psi_{\rho^*}^{(\lambda^*)E}$ up to a phase factor θ_ρ. If $\lambda^* \neq \lambda$, we have

$$\hat{T}\psi_\rho^{(\lambda)E} = \theta_\rho \psi_{\rho^*}^{(\lambda^*)E}, \qquad \text{for irreps of type } c. \tag{8-168a}$$

For the irreps of types a (with even N) and b (with odd N), $\lambda^* = \lambda$, and due to the assumption of no accidental degeneracy, from (8-167b) we have

$$\hat{T}\psi_\rho^{(\lambda)E} = \theta_\rho \psi_{\rho^*}^{(\lambda)E}, \qquad \text{for type } a \text{ (even } N) \text{ and } b. \tag{8-169a}$$

The two states $(\psi_\rho^{(\lambda)E}, \psi_{\rho^*}^{(\lambda)E})$ carry a two–dimensional representation of $\mathbf{T}$ with the matrix

$$D(\hat{T}) = \begin{pmatrix} 0 & \theta_{\rho^*} \\ \theta_\rho & 0 \end{pmatrix}.$$

In order that $D(\hat{T})^2 = +\mathbf{I}$ $(-\mathbf{I})$ for single–valued (double–valued) representations, it is necessary that

$$\theta_{\rho^*} = \pm\theta_\rho, \quad \text{for} \begin{cases} \text{type } a \text{ (single–valued)} \\ \text{type } b \text{ (double–valued)} \end{cases}. \tag{8-169b}$$

For type a irreps with odd N, which occur only for the one–dimensional irrep $\frac{n}{2}$ of the cyclic group C_n (including C_1, with no spatial symmetry at all), we have

$$\hat{T}\psi^E = \phi^E, \qquad \hat{T}\phi^E = -\psi^E, \quad \text{for double–valued type } a. \tag{8-168c}$$

This is the Kramers' theorem in its original form. The two states ψ^E and ϕ^E belong to the same irrep and are always orthogonal, since according to (8-163d) and $\hat{T}^2 = -1$ we have

$$\langle \psi^E | \hat{T}\psi^E \rangle = \langle \hat{T}\hat{T}\psi^E | \hat{T}\psi^E \rangle = -\langle \psi^E | \hat{T}\psi^E \rangle.$$

For example, $\psi^E = |j\tfrac{n}{2}\rangle$ and $\phi^E = |j - \tfrac{n}{2}\rangle$ are orthogonal.

From (8-168) and (8-169a) we can conclude that (compare with p. 12 of Koster 1963): the time reversal symmetry doubles the degeneracy of an eigenenergy E_λ if λ is an irrep of type a (N = odd) or type c (N = odd or even), but does not lead to any additional degeneracy if λ is an irrep of type a with even N or type b with odd N.

The reason for the above conclusions can also be understood in the following way: Under time reversal the states of type a (odd N) and type c will be shifted from one irreducible space to another, while the states of type a (even N) and type b will remain in the same irreducible space.

The dependence of the degeneracy of E_λ on irrep type a, b, c and number of fermions is listed in Table 8.13. Notice that the single–valued type c is possible only for one–dimensional irreps of the cyclic group C_n and the tetrahedral group T.

Table 8.13. Degeneracy of E_λ versus irrep types a,b,c and number of fermions, N.

	even N		odd N		
type	a	c	a	b	c
degeneracy	h_λ	2	2	h_λ(=even)	$2h_\lambda$

8.13.5. The transformation of the irreducible basis under time reversal

It is to be noted that in the case with multiplicity and if the multiplicity label $\bar{m}$ is chosen arbitrarily, the irreducible basis $\psi_\rho^{(\lambda)\bar{m}}$ for irreps of type a with even N and type b with odd N in general do not transform as shown in (8-169a). Instead, one only has

$$\hat{T}\psi_\rho^{(\lambda)\bar{m}} = \sum_{\bar{m}'} c_{\bar{m}'\rho}\psi_{\rho^*}^{(\lambda)\bar{m}'}.$$

However with suitable choice of multiplicity label we can always have

$$\hat{T}\psi_\rho^{(\lambda)\bar{m}} = \theta_\rho\psi_{\rho^*}^{(\lambda)\bar{m}}, \qquad \text{for type } a \text{ (even } N\text{) and } b. \tag{8-170a}$$

The SAF's obeying (8-170a) are said to be *T–symmetrized.* For example, if

$$\hat{T}\phi_\rho^{(\lambda)} = \theta_\rho\psi_{\rho^*}^{(\lambda)}.$$

then

$$\varphi_\rho^{(\lambda)\pm} = (\pm 1)^{1/2}\left(\psi_\rho^{(\lambda)} \pm \phi_\rho^{(\lambda)}\right)$$

is *T–symmetrized*,

$$\hat{T}\varphi_\rho^{(\lambda)\pm} = \theta_\rho \varphi_{\rho^*}^{(\lambda)\pm}.$$

If a SAF transforms as (8-170a), then its expansion coefficients have the symmetry

$$\langle j\,-m|\psi_{\rho^*}^{(\lambda)}\rangle = \theta_\rho(-1)^{j+m}\langle jm|\psi_\rho^{(\lambda)}\rangle^*.$$

Therefore the symmetrization procedure introduced an ad hoc manner by Chen & Fan (1999b) for obtaining the $T \supset C_3$ SAF's with multiplicity, is actually the *T–symmetrization*. After the *T–symmetrization* not only can the SAF's be more efficiently tabulated, but the numerical coefficients themselves become much simpler.

It is interesting to compare the irreps of the s–v type *a* and d–v type *b*. Both irreps are self time–reversed, that is $\psi_\rho^{(\lambda)}$ and $\hat{T}\psi_\rho^{(\lambda)}$ belong to the same irrep, but they have the following distinction: For irreps of s–v type *a*, the subgroup can be chosen so that ρ is real and thus so that each partner of the irrep is self time–reversed,

$$\hat{T}\varphi_\rho^{(\lambda)} = \varphi_\rho^{(\lambda)}, \qquad \text{for type } a \text{ even } N. \tag{8-170b}$$

However, for type *b* irreps only a pair of states $(\varphi_\rho^{(\lambda)}, \varphi_{\rho^*}^{(\lambda)})$ is self time–reversed, $\hat{T}\varphi_\rho^{(\lambda)} = \varphi_{\rho^*}^{(\lambda)}$, rather than any individual state. Notice that the states of type *b* always appear pair–wise with the two states in a pair being time–reversals of each other. Consequently, the dimension of an irrep of type *b* is necessarily even.

It is also interesting to notice the distinction between the s–v type *a* and d–v type *a*.

Single–valued type a :

For the group C_n, n = even, the states $|j, \frac{n}{2}\rangle$ and $|j, -\frac{n}{2}\rangle$ of the irrep $\frac{n}{2}$ can be linearly combined into $|j, \frac{n}{2}\rangle \pm |j, -\frac{n}{2}\rangle$ which are self time–reversed.

Double–valued type a :

For the group C_n, n = odd, the states $|j, \frac{n}{2}\rangle$ and $|j, -\frac{n}{2}\rangle$ for the irrep $\frac{n}{2}$ can not be linearly combined into a self time–reversed state.

Irreps of type *c* are not self time–reversed, but they always appear pair–wise with the two irreps in a pair being time–reversals of each other. Therefore the number of the irreps of type *c* of any group G is necessarily even.

As examples, we give the time reversal of the SAF's given in Sec. 8.5, 8.7 and 8.12. The SAF's given there hold also for many–electron cases, so long as the angular momentum j is interpreted as the total angular momentum of the N–electron system.

For the one–dimensional SAF's of D_n in (8-49a) and (8-158a):

$$\hat{T}\psi^{(A_{\rho\nu})\bar{m}} = (-1)^{-\bar{m}}\nu\psi^{(A_{\rho\nu^*})\bar{m}}. \tag{8-171a}$$

For the $D_n \supset C_n$ SAF's in (8-49c) and (8-158b):

$$\hat{T}\psi_\mu^{(E_\mu)\bar{m}} = (-1)^{\bar{m}+\xi}\psi_{-\mu}^{(E_\mu)\bar{m}},\ \mu > 0, \quad \xi = \begin{cases} 0, & \text{for s–v reps} \\ \frac{1}{2}, & \text{for d–v reps} \end{cases}. \tag{8-171b}$$

For the $D_n \supset C_{2x}$ SAF's in (8-49d) and (8-158c):

$$\begin{aligned} &\text{s–v (type a)} \qquad \hat{T}\psi_\nu^{(E_\mu)\bar{m}} = (-1)^{\bar{m}}\nu\psi_\nu^{(E_\mu)\bar{m}},\ \nu = \pm 1, \\ &\text{d–v (type b)} \qquad \hat{T}\psi_i^{(E_\mu)\bar{m}} = (-1)^{\bar{m}}\psi_{-i}^{(E_\mu)\bar{m}} \end{aligned} \tag{8-171c}$$

that is, the states $\psi_{\pm 1}^{(E_\mu)\bar{m}}$ are self time–reversed, and thus belong to the type a, while the states $\psi_{\pm i}^{(E_\mu)\bar{m}}$ are time–reversals of each other, and belong to the type b.

For the $T \supset C_3$ SAF's in (8-69a,b):

$$\begin{aligned} \hat{T}\psi_{\mu}^{(\Gamma)\bar{m}} &= (-1)^{l-\bar{m}}\mathrm{sign}(\bar{m})\psi_{-\mu}^{(\Gamma)\bar{m}}, \ \Gamma = A_0, F, \quad \text{type } a \\ \hat{T}\psi^{(A_\mu)\bar{m}} &= (-1)^{l-\bar{m}}\psi^{(A_{-\mu})-\bar{m}}, \quad \text{type } c\,. \end{aligned} \tag{8-172}$$

To illustrate equation (8-170b) we now list the $T \supset D_2$ SAF's (with the coordinate system as shown in Fig. 8.2-3) (Chen & Fan 1999b) and resultants after acting with time–reversal on those SAF's:

1. One–dimensional irrep

$$\begin{aligned} \varphi^{(A_\mu)\bar{m}} = {} & |Y_{l\bar{m}}\rangle + (-)^l|Y_{l,-\bar{m}}\rangle + (1+(-)^l)\left[\rho_\mu^* i^{\bar{m}} + \rho_\mu\right] d^l_{0\bar{m}}(\tfrac{\pi}{2})|Y_{l0}\rangle \\ & + 2\sum_{m=2,4,6,\cdots}\left[\rho_\mu^* i^{\bar{m}} + \rho_\mu i^m\right] d^l_{m\bar{m}}(\tfrac{\pi}{2})\left[|Y_{lm}\rangle + (-)^l|Y_{l,-m}\rangle\right], \\ & \bar{m} = \text{even}, \ \mu = 0, \pm 1, \ \rho_\mu = \exp(-\tfrac{2\pi\mu i}{3}). \end{aligned} \tag{8-173a}$$

It is noted that the SAF $\varphi^{(A_0)}$ is real, while $\varphi^{(A_1)} = (\varphi^{(A_{-1})})^*$, that is under the time reversal $\hat{T}$ we have

$$\hat{T}\varphi^{(A_0)} = \varphi^{(A_0)}, \ \hat{T}\varphi^{(A_1)} = (\varphi^{(A_1)})^* = \varphi^{(A_{-1})}. \tag{8-173b}$$

2. Three–dimensional irrep

$$\left\{\begin{array}{rcl} \varphi_x^{(F)\bar{m}} & = & i^{\bar{m}}\displaystyle\sum_{m=1,3,5,\cdots} d^l_{m\bar{m}}(\tfrac{\pi}{2})\left[|Y_{lm}\rangle + (-)^l|Y_{l,-m}\rangle\right], \\ \varphi_y^{(F)\bar{m}} & = & -\displaystyle\sum_{m=1,3,5,\cdots} i^m d^l_{m\bar{m}}(\tfrac{\pi}{2})\left[|Y_{lm}\rangle - (-)^l|Y_{l,-m}\rangle\right], \quad \bar{m} = \text{even} \\ \varphi_z^{(F)\bar{m}} & = & |Y_{l\bar{m}}\rangle - (-)^l|Y_{l,-\bar{m}}\rangle, \end{array}\right. \tag{8-174a}$$

The SAF $\varphi^{(F)}$ is real, and thus

$$\hat{T}\varphi_k^{(F)} = \varphi_k^{(F)}, \ k = x, y, z, \qquad \text{type } a, \tag{8-174b}$$

that is, the states $\varphi_k^{(F)}$ are self time–reversed.

Chapter 9

Applications of Group Theory to Many–Body Systems

Group theory plays a significant role in treating many–body systems. In this chapter we shall restrict ourselves to its applications in the nuclear shell model (both for pure and mixed configurations), the quark model, the dynamic symmetry model of nuclei and the molecular shell model. We only sketch the bare bones, leaving details to the references.

In Secs. 9.1–9.4 we use a round bracket $|\ )$ to denote a totally anti–symmetric state, and an angular bracket $|\ \rangle$ to indicate a state with arbitrary symmetry.

9.1. Nuclear Shell Model: Single–Shell

The nuclear many–body problem is notorious for its difficulty. It is difficult because nuclei consist of strongly interacting particles whose number is neither so small that exact calculation is possible nor large enough for statistical techniques to be applicable. Consequently, model theories play a decisive role in understanding the nuclei. The shell model underpins microscopic models of nuclei. Its basic idea is that, as a first approximation, nucleons can be described as moving independently in an average field provided by all other nucleons. The average field produces an infinite series of single particle levels $nljm$ exhibiting a shell structure, where n is the principal quantum number and $\mathbf{j} = \mathbf{l} + \frac{\mathbf{1}}{\mathbf{2}}$. The correlation between the particles is established through the action of some type of residual force. The residual interaction has two important ingredients, the short–range force and long–range force. The former favors a spherical shape for nuclei while the latter favors a deformed shape. The main features of the spectroscopy of low–lying nuclei can be accounted qualitatively by the interplay of these two kinds of residual interactions. However, detailed quantitative calculation is extremely difficult due to the huge dimension of the Hilbert space one meets as soon as many valence nucleons are present. Therefore the shell model calculation was restricted to light nuclei (the $1p$, $2s, 1d$ and $2p, 1f$ shell nuclei) and a very few nuclei in the vicinity of double magic nuclei. But with the rapid growth in computational power, the shell model calculation has undergone a revitalization and tremendous developments have been made. Effective diagonalization of the shell model Hamiltonian in model space with dimensions in the millions have become feasible (Pan 1996). Impressive developments have been made in the Quantum Monte Carlo method for the shell model, and model spaces with dimension 10^{10} can be handled (Honma 1996).

One of the key problems in the shell model is how to calculate the matrix elements of the Hamiltonian. We will discuss this problem in two cases, the single–shell and multi–shell cases. For single–shell we use both the first quantization and generalized quantization formalisms. There is little difference between the two as far as the single–shell is concerned, but for multi–shell the latter is superior than the former.

9.1.1. First quantization

It is convenient to use the abbreviation that $\rho = lst, \Gamma = \alpha L \beta S T$ for l–s coupling and $\rho = jt, \Gamma = \alpha J T$ for j–j coupling. The following conventions are also used for j–j coupling

$$(-1)^{\Gamma} = (-1)^{J+T} , \quad (-1)^{\rho} = (-1)^{j+t} , \tag{9-1}$$

with similar relations holding for the l–s coupling. The convention (7-175f) will still be used.

Let $Q^{\Gamma_0}(n_2)$ be a n_2–body operator. For example, in the l–s coupling, a general one–body operator is

$$Q(1)^{J_0 T_0} = \sum_{i=1}^{n} \left[U^{L_0}(i) V^{S_0}(i)\right]^{J_0}_{M_0} W^{T_0}_{M_{T_0}}(i) , \tag{9-2a}$$

and a rotationally invariant charge independent interaction is

$$Q(2) = \sum_{i>j=1}^{n} \left[U^{L_0}(ij) V^{L_0}(ij)\right]^{0}_{0} . \tag{9-2b}$$

From (7-175a), using the anti-symmetry property of the wave functions, and the fact that the operator $\mathcal{Q}^{\Gamma_0}(n_2)$ does not change the quantum numbers $[\nu_1]\Gamma_1$ of the first n_2 particles, we get the reduced matrix elements of the operator $Q^{\Gamma_0}(n_2)$,

$$\begin{aligned}
&\left(\rho^n[\bar{\nu}]\bar{\Gamma} \parallel Q^{\Gamma_0}(n_2) \parallel \rho^n[\nu]\Gamma\right) = \\
&\quad \binom{n}{n_2} \sum_{\nu_1 \bar{\nu}' \nu' \Gamma_1 \Gamma_2 \bar{\Gamma}_2} U(\Gamma_1 \rho \bar{\Gamma} \Gamma_0; \Gamma \rho)(\rho^{n_2}\bar{\Gamma}_2 \parallel \mathcal{Q}^{\Gamma_0}(n_2) \parallel \rho^{n_2}\Gamma_2) \\
&\quad \times \left(\rho^n[\bar{\nu}]\bar{\Gamma}\{|\rho^{n-n_2}[\nu_1]\Gamma_1, \rho^{n_2}\bar{\Gamma}_2\right)^{\bar{\nu}'} \left(\rho^{n-n_2}[\nu_1]\Gamma_1, \rho^{n_2}\Gamma_2|\}\rho^n[\nu]\Gamma\right)^{\nu'} ,
\end{aligned} \tag{9-3}$$

$$\mathcal{Q}^{\Gamma_0}(n_2) = \begin{cases} q^{\Gamma_0}(n), & n_2 = 1 \\ q^{\Gamma_0}(n-1, n), & n_2 = 2 , \end{cases}$$

where the indices $\bar{\nu}', \nu', \bar{\Gamma}_2$ and Γ_2 should be ignored when $n_2 = 1$, and the n_2–body CFP is given in (7-175b,d). Equation (9-3) is to be compared with (4.47) in Brussaard (1977). Notice that for the j–j coupling case, the partition $[\nu]$ is related to the total isospin as given in (7-54b), that is $[\tilde{\nu}] = [\frac{n}{2} + T, \frac{n}{2} - T]$, and thus can be ignored, as is done in Brussaard (1977).

It is seen that in terms of the n_2–body CFP, the evaluation of matrix elements of a n_2–body operator for a many–body system is reduced to that for a n_2–body system without the explicit form of the many–body wave functions.

9.1.2. Generalized quantization

For simplicity we use the j–j coupling with $\Gamma = \alpha J T$. For the l–s coupling, we need only interpret αJ as αL, and T as $\beta S T$. We begin with the introduction of the second quantized forms for the one– and two–body operators

$$Q^{\Gamma}_{\mu} = \sum_{\rho_1, \rho_2} \frac{\hat{\rho}_1}{\hat{\Gamma}} (\rho_1 \parallel Q^{\Gamma} \parallel \rho_2)[C^{\dagger}_{\rho_1} \times \tilde{C}_{\rho_2}]^{\Gamma}_{\mu} , \tag{9-4a}$$

$$\begin{aligned}
V = \frac{1}{2}\sum_{i \neq j} V_{ij} = \sum_{\Gamma} \sum_{\rho_1 \leq \rho_2, \rho_3 \leq \rho_4} &([1^2]\rho_1\rho_2, \Gamma | V_{12} | [1^2]\rho_3\rho_4, \Gamma) \\
&\times N_{12}^{-1/2} N_{34}^{-1/2} [C^{\dagger}_{\rho_1} \times C^{\dagger}_{\rho_2}]^{\Gamma} \cdot [\tilde{C}_{\rho_3} \times \tilde{C}_{\rho_4}]^{\Gamma} ,
\end{aligned} \tag{9-4b}$$

where $N_{12} = 1 + \delta_{\rho_1\rho_2}$ and $|[1^2]\rho_1\rho_2, \Gamma\mu)$ is a normalized anti-symmetric state

$$|[1^2]\rho_1\rho_2, \Gamma\mu) = A^\dagger_{\Gamma\mu}(\rho_1\rho_2)|0\rangle \ , \quad A^\dagger_{\Gamma\mu}(\rho_1\rho_2) = N_{12}^{-1/2}\left[C^\dagger_{\rho_1} \times C^\dagger_{\rho_2}\right]^\Gamma_\mu \ . \tag{9-4c}$$

Let us consider the pure configuration $(\rho)^n$. Using (7-311) and (7-313), the matrix elements of the operators $C^\dagger C, C^\dagger C^\dagger \tilde{C}\tilde{C}$ can be determined once the matrix elements of the hybrid operators $a^\dagger a, a^\dagger a^\dagger \tilde{a}\tilde{a}$ have been calculated.

We first calculate the matrix elements of $a^\dagger_\rho$. We use ν, ν', ν'' to denote the symmetries of the system with $n, n-1, n-2$ particles, respectively.

Using (7-108), (7-299) and (7-302) we have

$$\begin{aligned}\left(\rho^n[\nu]\Gamma \, \|a^\dagger_\rho\| \, \rho^{n-1}[\nu']\Gamma'\right) &= \sum_{mm'} \sqrt{\frac{1}{h_\nu h_{\nu'}}} \Lambda^\nu_m \Lambda^{\nu'}_{m'} \\ &\times \langle [\nu], \alpha J \, \|a^\dagger_j\| \, [\nu'], \alpha' J'\rangle \langle [\tilde{\nu}], T \, \|a^\dagger_t\| \, [\tilde{\nu}'], T'\rangle \\ &= (\nu|b^\dagger|\nu')\langle [\nu]\Gamma \, \|a^\dagger_\rho\| \, [\nu']\Gamma'\rangle \ , \end{aligned} \tag{9-5a}$$

where $(\nu|b^\dagger|\nu')$ is the $U_{2M} \supset U_M \times U_2$ ISF given in (7-232),

$$(\nu|b^\dagger|\nu') = (\nu'|b|\nu) = C^{[1^n]\nu\tilde{\nu}}_{[1^{n-1}]\nu'\tilde{\nu}',[1]} = \Lambda^\nu_{\nu'}\sqrt{\frac{h_{\nu'}}{h_\nu}} \ , \tag{9-5b}$$

and

$$\langle [\nu]\Gamma \, \|a^\dagger_\rho\| \, [\nu']\Gamma'\rangle \equiv \langle [\nu]\alpha J \parallel a^\dagger_j \parallel [\nu']\alpha' J'\rangle \langle [\tilde{\nu}]T \parallel a^\dagger_t \parallel [\tilde{\nu}']T'\rangle \ . \tag{9-5c}$$

The factor $(\nu|b^\dagger|\nu')$ decouples the j-space from the t-space, and the creation operator $b^\dagger$ can be visualized as the operation of adding one box to both the Young diagrams $[\nu']$ and $[\tilde{\nu}']$.

Equation (9-5a) is just the total one-body CFP cast in the generalized quantization form. If t is the isospin, the $[\tilde{\nu}]$ is redundant, the CFP $\langle [\tilde{\nu}]T \parallel a^\dagger_t \parallel [\tilde{\nu}']T'\rangle$ equals to one , and (9-5a) becomes

$$([1^n][\nu]\alpha JT \parallel a^\dagger_{jt} \parallel [1^{n-1}][\nu']\alpha' J'T') = \Lambda^\nu_{\nu'}\sqrt{\frac{h_{\nu'}}{h_\nu}}([\nu]\alpha J \parallel a^\dagger_j \parallel [\nu']\alpha' J') \ , \tag{9-6a}$$

which is just (7-179).

For the case of identical nucleons, $T = T_{max} = \frac{n}{2}$, (9-6a) reduces to

$$(\rho^n\Gamma\{|\rho^{n-1}\Gamma') = \langle [1^n]\alpha J \parallel a^\dagger_j \parallel [1^{n-1}]\alpha' J'\rangle \ . \tag{9-6b}$$

If α is interpreted as the quantum number of Sp_{2j+1}, then $\langle [1^n]\alpha J \parallel a^\dagger_j \parallel [1^{n-1}]\alpha' J'\rangle$ are the $SU_{2j+1} \supset Sp_{2j+1} \supset SO_3$ ISF, that is, the total CFP for identical-nucleon systems.

By inserting the identity operator (7-300) between two adjacent hybrid operators, we can calculate the matrix elements of any product of creation and annihilation operators.

Pair-creation operator

$$\begin{aligned}&\left(\rho^n[\nu]\Gamma \parallel [a^\dagger_\rho \times a^\dagger_\rho]^{\Gamma_0} \parallel \rho^{n-2}[\nu'']\Gamma''\right) \\ &\quad = \sum_{\nu'}(\nu|b^\dagger b^\dagger|\nu'')_{\nu'}\langle [\nu]\Gamma \parallel [a^\dagger_\rho \times a^\dagger_\rho]^{\Gamma_0} \parallel [\nu'']\Gamma''\rangle^{\nu'} \ . \end{aligned} \tag{9-7a}$$

The matrix elements $(\nu|b^\dagger b^\dagger|\nu'')_{\nu'}$ can be calculated by factorization:

$$(\nu|b^\dagger b^\dagger|\nu'')_{\nu'} = (\nu|b^\dagger|\nu')(\nu'|b^\dagger|\nu'') = \Lambda^\nu_{\nu'}\Lambda^{\nu'}_{\nu''}\sqrt{\frac{h_{\nu''}}{h_\nu}} \ , \tag{9-7b}$$

while

$$\langle [\nu]\Gamma \parallel [a_\rho^\dagger \times a_\rho^\dagger]^{\Gamma_0} \parallel [\nu'']\Gamma'' \rangle^{\nu'} \equiv \langle [\nu]\alpha J \parallel [a_j^\dagger \times a_j^\dagger]^{J_0} \parallel [\nu'']\alpha'' J'' \rangle^{\nu'} \langle [\tilde{\nu}]T \parallel [a_t^\dagger \times a_t^\dagger]^{T_0} \parallel [\tilde{\nu}'']T'' \rangle^{\tilde{\nu}'} . \tag{9-7c}$$

The matrix elements $\langle [\nu]\alpha J \parallel [a_j^\dagger \times a_j^\dagger]^k \parallel [\nu'']\alpha'' J'' \rangle^{\nu'}$ have been given in (7-308). Equation (9-7a) is just the combination of (7-181) and (7-176).

One-body operator

$$(\rho^n[\bar{\nu}]\bar{\Gamma} \parallel [a_\rho^\dagger \times \tilde{a}_\rho]^{\Gamma_0} \parallel \rho^n[\nu]\Gamma) = \sum_{\nu'} (\bar{\nu}|b^\dagger b|\nu)_{\nu'} \langle [\bar{\nu}]\bar{\Gamma} \parallel [a_\rho^\dagger \times \tilde{a}_\rho]^{\Gamma_0} \parallel [\nu]\Gamma \rangle^{\nu'} , \tag{9-8a}$$

$$(\bar{\nu}|b^\dagger b|\nu)_{\nu'} = (\bar{\nu}|b^\dagger|\nu')(\nu'|b|\nu) = \Lambda_{\nu'}^{\bar{\nu}} \Lambda_{\nu'}^{\nu} \frac{h_{\nu'}}{\sqrt{h_{\bar{\nu}} h_\nu}} . \tag{9-8b}$$

The matrix elements of $[a_\rho^\dagger \times \tilde{a}_\rho]^{\Gamma_0}$ can be calculated using (7-308),

$$\langle [\bar{\nu}]\bar{\Gamma} \parallel [a_\rho^\dagger \times \tilde{a}_\rho]^{\Gamma_0} \parallel [\nu]\Gamma \rangle^{\nu'} = \sum_{\Gamma'} (-1)^{2\rho-\Gamma_0} U(\Gamma\rho\bar{\Gamma}\rho; \Gamma'\Gamma_0) \times \langle [\bar{\nu}]\bar{\Gamma} \parallel a_\rho^\dagger \parallel [\nu']\Gamma' \rangle \langle [\nu']\Gamma' \parallel \tilde{a}_\rho \parallel [\nu]\Gamma \rangle . \tag{9-8c}$$

The matrix elements of the creation and annihilation operators are related through

$$\langle [\nu']\Gamma' \parallel \tilde{a}_\rho \parallel [\nu]\Gamma \rangle = \frac{\hat{\Gamma}}{\hat{\Gamma}'} (-1)^{\Gamma'+\rho-\Gamma} \langle [\nu]\Gamma \parallel a_\rho^\dagger \parallel [\nu']\Gamma' \rangle , \tag{9-8d}$$

which is obtained with the help of

$$\langle a \parallel T_\lambda \parallel b \rangle = (-1)^{a+\lambda-b} \frac{\hat{b}}{\hat{a}} \langle b \parallel T_\lambda^\dagger \parallel a \rangle^* .$$

For j–j coupling case, there is no summation over T' in (9-8c), since it is uniquely dictated by ν'.

Two-body operator

$$V(\rho) = [a_\rho^\dagger \times a_\rho^\dagger]^{\Gamma_2} \cdot [\tilde{a}_\rho \times \tilde{a}_\rho]^{\Gamma_2} ,$$

where the scalar product is defined by

$$T^k \cdot U^k = (-1)^k \sqrt{2k+1} [T^k \times U^k]_0^0 .$$

The matrix elements of $V(\rho)$ are

$$\left(\rho^n[\bar{\nu}]\bar{\Gamma} \parallel V(\rho) \parallel \rho^n[\nu]\Gamma\right) = \sum_{\bar{\nu}'\nu''\nu'} (\bar{\nu}|b^\dagger b^\dagger bb|\nu)_{\bar{\nu}'\nu''\nu'} \langle [\bar{\nu}]\bar{\Gamma} \parallel V(\rho) \parallel [\nu]\Gamma \rangle^{\bar{\nu}'\nu''\nu'} , \tag{9-9a}$$

where

$$(\bar{\nu}|b^\dagger b^\dagger bb|\nu)_{\bar{\nu}'\nu''\nu'} = (\bar{\nu}|b^\dagger b^\dagger|\nu'')_{\bar{\nu}'} (\nu''|bb|\nu)_{\nu'} = \Lambda_{\bar{\nu}'}^{\bar{\nu}} \Lambda_{\nu''}^{\bar{\nu}'} \Lambda_{\nu'}^{\nu'} \Lambda_{\nu'}^{\nu} \frac{h_{\nu''}}{\sqrt{h_{\bar{\nu}} h_\nu}} , \tag{9-9b}$$

$$\langle [\bar{\nu}]\bar{\Gamma} \parallel V(\rho) \parallel [\nu]\Gamma \rangle^{\bar{\nu}'\nu''\nu'} = \sum_{\alpha''\Gamma''} (-1)^{\Gamma''-\Gamma} \times (\hat{\Gamma}''/\hat{\Gamma}) \langle [\bar{\nu}]\bar{\Gamma} \parallel [a_\rho^\dagger \times a_\rho^\dagger]^{\Gamma_2} \parallel [\nu'']\Gamma'' \rangle^{\bar{\nu}'} \langle [\nu'']\Gamma'' \parallel [\tilde{a}_\rho \times \tilde{a}_\rho]^{\Gamma_2} \parallel [\nu]\Gamma \rangle^{\nu'} , \tag{9-9c}$$

with the matrix elements of the pair annihilation operator related to those of the pair creation operator by

$$\langle [\nu'']\Gamma'' \,\|[\tilde{a}_\rho \times \tilde{a}_\rho]^{\Gamma_2}\|\, [\nu]\Gamma\rangle^{\nu'} = \frac{\hat{\Gamma}}{\hat{\Gamma}''}(-1)^{\Gamma''+\Gamma_2-\Gamma}\langle [\nu]\Gamma \,\|[a_\rho^\dagger \times a_\rho^\dagger]^{\Gamma_2}\|\, [\nu'']\Gamma''\rangle^{\nu'} \,. \tag{9-9d}$$

Note that there is no summation over T'' in (9-9c) for j–j coupling.

Using (7-311), (9-4a) and (9-8) we can find the matrix elements of the one–body operator

$$\begin{aligned}(\rho^n[\bar{\nu}]\bar{\Gamma} \,\|\, Q^{\Gamma_0} \,\|\, \rho^n[\nu]\Gamma) &= n\frac{\hat{\rho}}{\hat{\Gamma}_2}(\rho \,\|\, q^{\Gamma_0} \,\|\, \rho)\left(\rho^n[\bar{\nu}]\bar{\Gamma} \,\|\, [a_\rho^\dagger \times \tilde{a}_\rho]^{\Gamma_0} \,\|\, \rho^n[\nu]\Gamma\right) \\ &= n\sum_{\nu'\Gamma'}(\rho \,\|\, Q^{\Gamma_0} \,\|\, \rho)(\bar{\nu}|b^\dagger b|\nu)_{\nu'}U(\Gamma'\rho\bar{\Gamma}\Gamma_0;\Gamma\rho)\langle[\bar{\nu}]\bar{\Gamma} \,\|\, a_\rho^\dagger \,\|\, [\nu']\Gamma'\rangle\langle[\nu]\Gamma \,\|\, a_\rho^\dagger \,\|\, [\nu']\Gamma'\rangle \,,\end{aligned} \tag{9-10}$$

which is just (9-3) with $n_2 = 1$.

Using (7-313), (9-4b) and (9-9) we can find the the matrix elements of two-body operators

$$\begin{aligned}(\rho^n[\bar{\nu}]\bar{\Gamma} \,\|\, V \,\|\, \rho^n[\nu]\Gamma) &= \binom{n}{2}\sum_{\Gamma_2}(\rho^2\Gamma_2 \,\|\, V_{12} \,\|\, \rho^2\Gamma_2) \\ &\times \left(\rho^n[\tilde{\nu}] \,\|\, \left[a_\rho^\dagger \times a_\rho^\dagger\right]^{\Gamma_2} \cdot [\tilde{a}_\rho \times \tilde{a}_\rho]^{\Gamma_2} \,\|\, \rho^n[\nu]\Gamma\right) \\ &= \binom{n}{2}\sum_{\bar{\nu}'\nu''\nu'\Gamma_2\Gamma'}(\rho^2\Gamma_2 \,\|\, V_{12} \,\|\, \rho^2\Gamma_2)\sum_{\bar{\nu}'\nu''\nu'}(\bar{\nu}|b^\dagger b^\dagger bb|\nu)_{\bar{\nu}'\nu''\nu'} \\ &\times \langle[\bar{\nu}]\bar{\Gamma} \,\|\, [a_\rho^\dagger \times a_\rho^\dagger]^{\Gamma_2} \,\|\, [\nu'']\Gamma''\rangle^{\bar{\nu}'}\langle[\nu]\Gamma \,\|\, [a_\rho^\dagger \times a_\rho^\dagger]^{\Gamma_2} \,\|\, [\nu'']\Gamma''\rangle^{\nu'} \,,\end{aligned} \tag{9-11}$$

which is just (9-3) with $n_2 = 2$ and $\Gamma_0 = 0$.

It is seen that the role played by the permutation group is to provide the intermediate quantum numbers, ν' for the single–body operator, and $\bar{\nu}'\nu''\nu'$ for the two–body operator, specifying the path for the factorization of the matrix elements.

9.2. Nuclear Shell Model: Multi–Shell*

There are two possible ways of treating the multi–j cases. The first uses the procedure of first anti–symmetrizing each single (jt) space and then anti–symmetrizing the total space. This is represented by the scheme:

$$\left|[1^n]\left(\ldots(\rho_1^{n_1}[1^{n_1}]J_1T_1\,,\rho_2^{n_2}[1^{n_2}]J_2T_2)J_{12}T_{12}\ldots JT\right)\right\rangle, \qquad n = n_1 + n_2 + \ldots \,.$$

The Oak Ridge code (French 1983) and Ritsschil code (Zwart 1985) use this scheme. Tutorial monographs on this approach are available (Brussaard 1977, De–Shalit 1963). An alternative method is to couple successive wave functions in each configuration $(j_i)^{n_i}$ with permutation symmetry $[\nu_i]$ to a total symmetry $[\nu]$, and then couple it to the wave function in the isospin space. This is represented by the scheme

$$\left|[1^n]\left(\ldots(j_1^{n_1}[\nu_1]J_1, j_2^{n_2}[\nu_2]J_2)[\nu_{12}]J_{12}\ldots[\nu]J\right);(t)^n[\tilde{\nu}]T\right\rangle \,.$$

The first scheme has a simpler formalism than the second scheme, but it also requires more storage space and computing time than the second. A code DUSM based on the second scheme is available (Vallieres 1994), and has proven very efficient. In this section, we will treat the two-shell case using the second scheme. Based on the two–shell formalism a recursive algorithm can be set up for the multi–shell case. Such an algorithm is embedded in the DUSM code.

Consider the configuration $j_1^{n_1} j_2^{n_2}$. Let $2j_i + 1 = N_i, N = N_1 + N_2$. The $SU_{2j+1} \supset SO_3$ basis $|[\nu]\alpha J\rangle$ is extended to the $SU_N \supset \Big(\big(SU_{N_1} \supset SO_3\big) \otimes \big(\big(SU_{N_2} \supset SO_3\big)\Big) \supset SO_3$ basis,

$$|[\nu]\theta, \nu_1 J_1 \nu_2 J_2; J\rangle \ ,$$

and the one-body CFP $\langle [\nu]\alpha J \, \|a_i^\dagger\| \, [\nu']\alpha' J'\rangle$ are extended to

$$\langle [\nu]\theta, \nu_1 J_1 \nu_2 J_2; J \, \|a_j^\dagger\| \, [\nu']\theta', \nu_1' J_1' \nu_2' J_2'; J'\rangle \ , \tag{9-12}$$

where $\theta = 1, 2, \ldots \{\nu_1 \nu_2 \nu\}$ is the multiplicity label. Equation (9-12) represents the one-body CFP for the two-shell state, namely the $SU_N \supset \Big(\big(SU_{N_1} \supset SO_3\big) \otimes \big(SU_{N_2} \supset SO_3\big)\Big) \supset SO_3$ ISF.

The CFP expansion of a two-shell state is

$$\begin{aligned} |[\nu]\theta, \nu_1 J_1 \nu_2 J_2; J\rangle = \sum_{i=1,2} \sum_{\nu_1' J_1' \nu_2' J_2' J'} & \langle [\nu]\theta, \nu_1 J_1 \nu_2 J_2; J \, \|a_{j_i}^\dagger\| \, [\nu']\theta', \nu_1' J_1' \nu_2' J_2'; J'\rangle \\ & \times \Big[\Big|[\nu']\theta', \nu_1' J_1' \nu_2' J_2'; J'\Big\rangle \, \psi_{j_i}(n)\Big]^J \ . \end{aligned} \tag{9-13}$$

According to the factorization lemma, the ISF in (9-12) can be factorized into a $SU_N \supset SU_{N_1} \otimes SU_{N_2}$ ISF and the remaining part,

$$\begin{aligned} & \langle [\nu]\theta, \nu_1 J_1 \nu_2 J_2; J \, \|a_{j_i}^\dagger\| \, [\nu']\theta', \nu_1' J_1' \nu_2' J_2'; J'\rangle \\ & \quad = \langle \nu_1 \nu_2, \nu\theta | a_i^\dagger | \nu_1' \nu_2', \nu'\theta'\rangle \langle \nu_1 J_1 \nu_2 J_2; J \, \|a_{j_i}^\dagger\| \, \nu_1' J_1' \nu_2' J_2'; J'\rangle \ , \end{aligned} \tag{9-14a}$$

where the $\langle \nu_1 \nu_2, \nu\theta | a_i^\dagger | \nu_1' \nu_2', \nu'\theta'\rangle$ are the $SU_N \supset SU_{N_1} \otimes SU_{N_2}$ ISF, or the $S_n \supset S_{n-1}$ outer-product ISF. With the old notation and $i = 1$ it is

$$\begin{aligned} \langle \nu_1 \nu_2, \nu\theta | a_1^\dagger | \nu_1' \nu_2, \nu'\theta'\rangle &= \langle \nu_1' \nu_2, \nu'\theta' | a_1 | \nu_1 \nu_2, \nu'\theta'\rangle \\ &= C^{[\nu]\theta, \nu_1 \nu_2}_{[\nu']\theta' \nu_1' \nu_2, [1][1][0]} = C^{[\nu]\theta, [\nu]\theta}_{\nu_1 \nu_1', \nu_2 \nu_2} \ . \end{aligned} \tag{9-14b}$$

A similar equation holds for $i = 2$. The outer-product ISF decouples the first and second shells, while the second factor on the right hand side of (9-14a) can be calculated using the Racah algebra,

$$\langle \nu_1 J_1 \nu_2 J_2; J \, \|a_{j_1}^\dagger\| \, \nu_1' J_1' \nu_2' J_2'; J'\rangle = \delta_{\nu_2 \nu_2'} \delta_{J_2 J_2'} \langle [\nu_1] J_1 \, \|a_{j_1}^\dagger\| \, [\nu_1'] J_1'\rangle \begin{pmatrix} J_1' & J_2 & J' \\ j_1 & 0 & j_1 \\ J_1 & J_2 & J \end{pmatrix} \ . \tag{9-14c}$$

The one-body matrix elements $\langle [\bar{\nu}]\bar{\alpha}\bar{J} \, \|[a_j^\dagger \times \tilde{a}_j]^{J_0}\| \, [\nu]\alpha J\rangle^{\nu'}$ are replaced by

$$\begin{aligned} & \langle [\bar{\nu}]\bar{\theta}, \bar{\nu}_1 \bar{J}_1 \bar{\nu}_2 \bar{J}_2; \bar{J} \, \|[a_{j_i}^\dagger \times \tilde{a}_{j_k}]^{J_0}\| \, [\nu]\theta, \nu_1 J_1 \nu_2 J_2; J\rangle^{\nu'} \\ & \quad = \sum_{(\nu_1 \nu_2)_{\text{int}}} \langle \bar{\nu}_1 \bar{\nu}_2, \bar{\nu}\bar{\theta} | a_i^\dagger a_k | \nu_1 \nu_2, \nu\theta\rangle^{\nu'}_{(\nu_1 \nu_2)_{\text{int}}} \\ & \quad \times \langle \bar{\nu}_1 \bar{J}_1 \bar{\nu}_2 \bar{J}_2; \bar{J} \, \|[a_{j_i}^\dagger \times \tilde{a}_{j_k}]^{J_0}\| \, \nu_1 J_1 \nu_2 J_2, J\rangle^{(\nu_1 \nu_2)_{\text{int}}} \ , \end{aligned} \tag{9-15}$$

where $(\nu_1 \nu_2)_{\text{int}}$ is the shorthand notation for the irrep label of the intermediate states, which specify the path for the factorization of the two matrix elements. The first matrix elements, $\langle \bar{\nu}_1 \bar{\nu}_2, \bar{\nu}\bar{\theta} | a_i^\dagger a_k | \nu_1 \nu_2, \nu\theta\rangle$, undo the coupling between shells 1 and 2 at the unitary group level.

By inserting a complete set of intermediate states and noting that the quantum numbers ν' and $(\nu_1\nu_2)_{\rm int}$ have already specified the irrep labels of the intermediate states, we have

$$\langle\bar{\nu}_1\nu_2,\bar{\nu}\bar{\theta}|a_1^\dagger a_1|\nu_1\nu_2,\nu\theta\rangle^{\nu'}_{\nu'_1} = \sum_{\theta'}\langle\bar{\nu}_1\nu_2,\bar{\nu}\bar{\theta}|a_1^\dagger|\nu'_1\nu_2,\nu'\theta'\rangle\langle\nu'_1\nu_2,\nu'\theta'|a_1|\nu_1\nu_2,\nu\theta\rangle$$

$$\langle\nu_1^0\nu'_2,\bar{\nu}\bar{\theta}|a_1^\dagger a_2|\nu_1\nu_2,\nu\theta\rangle^{\nu'} = \sum_{\theta'}\langle\nu_1^0\nu'_2,\bar{\nu}\bar{\theta}|a_1^\dagger|\nu_1\nu'_2,\nu'\theta'\rangle\langle\nu_1\nu'_2,\nu'\theta'|a_2|\nu_1\nu_2,\nu\theta\rangle$$

$$\langle\nu'_1\nu_2^0,\bar{\nu}\bar{\theta}|a_2^\dagger a_1|\nu_1\nu_2,\nu\theta\rangle^{\nu'} = \sum_{\theta'}\langle\nu'_1\nu_2^0,\bar{\nu}\bar{\theta}|a_2^\dagger|\nu'_1\nu_2,\nu'\theta'\rangle\langle\nu'_1\nu_2,\nu'\theta'|a_1|\nu_1\nu_2,\nu\theta\rangle\ ,$$

where ν_i^0 is the irrep label of the group S_{n_i+1}.

The matrix elements $\langle\bar{\nu}_1\bar{J}_1\bar{\nu}_2\bar{J}_2;\bar{J}\ \|[a_{j_i}^\dagger\times\tilde{a}_{j_k}]^{J_0}\|\ \nu_1J_1\nu_2J_2;J\rangle^{(\nu_1\nu_2)_{\rm int}}$ in the decoupled basis can be calculated using the Racah algebra and will not be given here.

In a similar way, we can calculate the matrix elements of two–body operators. For more detail, the reader is referred to Chen (1991).

The extension from single spin to two–spin is as follows. Suppose we have the quark model in mind, then the basis vector $|[\nu]T\rangle$ is extended to the $SU_6\supset\left(SU_3^f\supset SU_2\otimes U_1\right)\times SU_2^s$ basis $|[\nu]\beta(\lambda\mu)IYS\rangle$, where we ignore the quantum numbers I_z,S_z. The one–body CFP $\langle[\nu]T\ \|a_t^\dagger\|\ [\nu']T'\rangle$ are replaced by the $SU_6\supset\left(SU_3\supset SU_2\otimes U_1\right)\times SU_2$ CFP,

$$\langle[\nu]\phi(\lambda\mu)IYS\ \|a^\dagger_{(10)\frac{1}{2}\frac{1}{2}}\|\ [\nu']\phi'(\lambda'\mu')I'Y'S'\rangle\ , \tag{9-16}$$

which can be factorized into a product of $SU_6\supset SU_3\times SU_2$ CFP and $SU_3\supset SU_2\otimes U_1$ CFP (see (7-156)),

$$\begin{aligned}&\langle[\nu]\phi(\lambda\mu)IYS\ \|a^\dagger_{(10)\frac{1}{2}\frac{1}{2}}\|\ [\nu']\phi'(\lambda'\mu')I'Y'S'\rangle\\ &\quad=\langle\nu_3\nu_s,\nu\phi|b^\dagger|\nu'_3\nu'_s,\nu'\phi'\rangle\langle(\lambda\mu)IY\ \|a^\dagger_{(10)\frac{1}{2}}\|\ (\lambda'\mu')I'Y'\rangle\ ,\end{aligned} \tag{9-17}$$

where $[\nu_3]\equiv[\lambda+\mu,\mu],[\nu_s]=[\frac{n}{2}+S,\frac{n}{2}-S],\phi=1,2,\ldots(\nu_3\nu_s\nu)$, and the $\langle\nu_3\nu_s,\nu\phi|b^\dagger|\nu'_3\nu'_s,\nu'\phi'\rangle$ are the $SU_6\supset SU_3\times SU_2$ ISF, or the $S_n\supset S_{n-1}$ ISF. With the old notation this is

$$\begin{aligned}\langle\nu_3\nu_s,\nu\phi|b^\dagger|\nu'_3\nu'_s,\nu'\phi'\rangle&=\langle\nu'_3\nu'_s,\nu'\phi'|b|\nu_3\nu_s,\nu\phi\rangle\\ &=C^{[\nu]\phi,\nu_3\nu_s}_{[\nu']\phi'\nu'_3\nu'_s,[1][1][1]}=C^{[\nu]\phi,[\nu']\phi'}_{\nu_3\nu'_3,\nu_s\nu'_s}\ .\end{aligned} \tag{9-18}$$

The $SU_6\supset SU_3\times SU_2$ ISF in (9-17) undo the coupling between the SU_3^f space and SU_2^s space. The matrix elements of one–body and two–body operators for the two–spin case are also given in Chen (1991).

The advantage of the present approach over the first quantization approach is that here we focus our attention solely on the reduced matrix elements without using any wave functions so that irreducible tensor techniques can be utilized in a straightforward manner.

9.3. Anti-Symmetric Wave Functions for an A + B System

Let A and B be two nuclei, or two shells in the same nucleus with f_1 and f_2 particles respectively and let $f=f_1+f_2$. The relevant quantum numbers for the systems A, B and A + B are shown in Table 9.2,

Table 9.2. Quantum numbers for nuclear systems A, B and A+B

	A	B	A + B
orbital angular momentum	L_1	L_2	L
spin	S_1	S_2	S
isospin	T_1	T_2	T
symmetry in orbital space	$[\nu_1]$	$[\nu_2]$	$[\nu]$
symmetry in spin space	$[\sigma_1]$	$[\sigma_2]$	$[\sigma]$
symmetry in isospin space	$[\mu_1]$	$[\mu_2]$	$[\mu]$

where

$$[\sigma_i] = \left[\tfrac{f_i}{2} + S_i, \tfrac{f_i}{2} - S_i\right], \quad [\sigma] = \left[\tfrac{f}{2} + S, \tfrac{f}{2} - S\right],$$
$$[\mu_i] = \left[\tfrac{f_i}{2} + T_i, \tfrac{f_i}{2} - T_i\right], \quad [\mu] = \left[\tfrac{f}{2} + T, \tfrac{f}{2} - T\right]. \tag{9-19}$$

The anti-symmetric wave functions of A and B are denoted by $\left|{}^{[\nu_i]}_{L_i\beta_i S_i T_i}\right)$ (see (7-171)). For brevity here and in what follows we often ignore the additional quantum number α_i and the projections M_{L_i}, M_{S_i} and M_{T_i}.

The anti-symmetric wave function for the total system A + B is then

$$\Psi_{LST} = \mathcal{A}\left[\left|\begin{matrix}[\nu_1]\\ L_1\beta_1 S_1 T_1\end{matrix}\right)_{\omega_1^0}\left|\begin{matrix}[\nu_2]\\ L_2\beta_2 S_2 T_2\end{matrix}\right)_{\omega_2^0} F(A-B)\right]^{LST}, \tag{9-20a}$$

where $(\omega_1^0) = (1, 2, \ldots, f_1)$ and $(\omega_2^0) = (f_1 + 1, \ldots, f)$. The function F(A–B) is equal to one if A and B represent two shells in a nucleus. It is equal to the relative motion wave function if A and B represent two nuclei in a nuclear reaction, or two clusters in the cluster model,

$$F(\mathrm{A} - \mathrm{B}) = F(\mathbf{R}_\mathrm{A} - \mathbf{R}_\mathrm{B}), \tag{9-20b}$$

with $\mathbf{R}_\mathrm{A}$ and $\mathbf{R}_\mathrm{B}$ being the positions of the mass centers of A and B. $\mathcal{A}$ is the anti-symmetrization operator, and can be expressed as

$$\mathcal{A} = \binom{f}{f_1}^{-1/2} \sum_\omega \delta_\omega \binom{\omega^0}{\omega}, \tag{9-20c}$$

where $\binom{\omega^0}{\omega}$ is the order-preserving operator [(4-131)], and δ_ω is it's permutation parity.

The form (9-20a) for the anti-symmetric wave function is not convenient for calculating matrix elements of the interactions between the two clusters A and B. Instead, we will construct the anti-symmetric wave function in the following way. First, in orbital space we construct the $SU_{m+n} \supset SU_m \otimes SU_n$ basis (if A and B represent two shells l_1 and l_2, then $m = 2l_1 + 1$ and $n = 2l_2 + 1$),

$$\left|\begin{matrix}[\nu] & \tau[\nu_1][\nu_2]\\ m, LM_L; & L_1\ L_2\end{matrix}\right\rangle$$
$$= \sum_{m_1 m_2 \omega} C^{[\nu]\tau,m}_{\nu_1 m_1, \nu_2 m_2, \omega}\binom{\omega^0}{\omega}\left[\left|\begin{matrix}[\nu_1]\\ m_1\omega_1^0, L_1\end{matrix}\right\rangle\left|\begin{matrix}[\nu_2]\\ m_2\omega_2^0, L_2\end{matrix}\right\rangle F(A-B)\right]^L_{M_L}. \tag{9-21}$$

Next, in spin–isospin space we construct the $SU_4 \supset SU_2 \times SU_2$ basis,

$$\left|\begin{matrix}[\tilde{\nu}]\\ \tilde{m}, \beta S T M_s M_T\end{matrix}\right\rangle = \sum_{m_\sigma m_\mu} C^{[\tilde{\nu}]\beta,\tilde{m}}_{[\sigma]m_\sigma,[\mu]m_\mu}\left|\begin{matrix}[\sigma]\\ m_\sigma, SM_s\end{matrix}\right\rangle\left|\begin{matrix}[\mu]\\ m_\mu, TM_T\end{matrix}\right\rangle. \tag{9-22a}$$

Finally we use (4-125) to form the totally anti-symmetric wave function

$$\left| \begin{matrix} [\nu] & \tau[\nu_1][\nu_2] \\ L\beta ST, & L_1\ L_2 \end{matrix} \right) = \sum_m \frac{\Lambda_m^\nu}{\sqrt{h_\nu}} \left| \begin{matrix} [\nu] & \tau[\nu_1][\nu_2] \\ m, L; & L_1\ L_2 \end{matrix} \right\rangle \left| \begin{matrix} [\tilde{\nu}] \\ \tilde{m}\beta ST \end{matrix} \right\rangle . \tag{9-22b}$$

The two anti-symmetric bases (9-20a) and (9-22b) are related by a unitary transformation

$$\begin{aligned} &\left| \begin{matrix} [\nu] & \tau[\nu_1][\nu_2] \\ L\beta ST, & L_1\ L_2 \end{matrix} \right) \\ &= \sum_{\substack{\beta_1 S_1 T_1 \\ \beta_2 S_2 T_2}} C^{[\tilde{\nu}]\tau,\beta ST}_{[\tilde{\nu}_1]\beta_1 S_1 T_1,[\tilde{\nu}_2]\beta_2 S_2 T_2} \mathcal{A} \left[\left| \begin{matrix} [\nu_1] \\ L_1\beta_1 S_1 T_1 \end{matrix} \right)_{\omega_1^0} \left| \begin{matrix} [\nu_2] \\ L_2\beta_2 S_2 T_2 \end{matrix} \right)_{\omega_2^0} F(A-B) \right]^{LST} . \end{aligned} \tag{9-22c}$$

Equation (9-22c) can be justified by noting that the $SU_4 \supset SU_2 \times SU_2$ ISF ensure that the spin–isospin wave functions on the right-hand side belong to the irrep $[\tilde{\nu}]$ of SU_4, while the anti-symmetrization operator ensures that the right-hand side of (9-22c) is totally anti-symmetric. Therefore the orbital wave function must have the symmetry $[\nu]$. From (7-154), the inverse of (9-22c) is

$$\begin{aligned} &\mathcal{A} \left[\left| \begin{matrix} [\nu_1] \\ L_1\beta_1 S_1 T_1 \end{matrix} \right)_{\omega_1^0} \left| \begin{matrix} [\nu_2] \\ L_2\beta_2 S_2 T_2 \end{matrix} \right)_{\omega_2^0} F(A-B) \right]^{LST} \\ &= \sum_{\nu\beta\tau} C^{[\tilde{\nu}]\tau,\beta ST}_{[\tilde{\nu}_1]\beta_1 S_1 T_1,[\tilde{\nu}_2]\beta_2 S_2 T_2} \left| \begin{matrix} [\nu] & \tau[\nu_1][\nu_2] \\ L\beta ST, & L_1\ L_2 \end{matrix} \right) . \end{aligned} \tag{9-23}$$

The extension to the $SU_6 \supset SU_2 \times SU_3$ case for hyper-nuclei is straightforward. All we have to do is to interpret $[\mu]$ in the above equations as the irrep label of SU_3, and T as IY, replace the spin–isospin wave function (9-22a) by the $SU_6 \supset SU_2 \times SU_3$ wave function

$$\left| \begin{matrix} [\tilde{\nu}] \\ \tilde{m}, \beta[\mu] IYI_z, SS_z \end{matrix} \right\rangle = \sum_{m_\sigma m_\mu} C^{[\tilde{\nu}]\beta,\tilde{m}}_{[\sigma]m_\sigma,[\mu]m_\mu} \left| \begin{matrix} [\sigma] \\ m_\sigma,\ SS_z \end{matrix} \right\rangle \left| \begin{matrix} [\mu] \\ m_\mu,\ IYI_z \end{matrix} \right\rangle , \tag{9-24a}$$

and replace (9-22b) with the expression

$$\left| \begin{matrix} [\nu] & \tau[\nu_1][\nu_2] \\ L\beta[\mu] IYS; & L_1\ L_2 \end{matrix} \right) = \sum_m \frac{\Lambda_m^\nu}{\sqrt{h_\nu}} \left| \begin{matrix} [\nu] & \tau[\nu_1][\nu_2] \\ m, L; & L_1\ L_2 \end{matrix} \right\rangle \left| \begin{matrix} [\tilde{\nu}] \\ \tilde{m}, \beta[\mu] IYS \end{matrix} \right\rangle . \tag{9-24b}$$

The generalization of (9-22c) and (9-23) are as follows:

$$\begin{aligned} &\left| \begin{matrix} [\nu] & \tau[\nu_1][\nu_2] \\ L\beta[\mu] IYS\ , & L_1\ L_2 \end{matrix} \right) = \sum_{\beta_1\mu_1 S_1 \beta_2\mu_2 S_2} C^{[\tilde{\nu}]\tau,\beta\mu S}_{[\tilde{\nu}_1]\beta_1\mu_1 S_1,[\tilde{\nu}_2]\beta_2\mu_2 S_2} \\ &\times \mathcal{A} \left[\left| \begin{matrix} [\nu_1] \\ L_1\beta_1[\mu_1] S_1 \end{matrix} \right\rangle_{\omega_1^0} \left| \begin{matrix} [\nu_2] \\ L_2\beta_2[\mu_2] S_2 \end{matrix} \right\rangle_{\omega_2^0} F(A-B) \right]^{L[\mu]S}_{IY} . \end{aligned} \tag{9-24c}$$

$$\begin{aligned} &\mathcal{A} \left[\left| \begin{matrix} [\nu_1] \\ L_1\beta_1[\mu_1] S_1 \end{matrix} \right)_{\omega_1^0} \left| \begin{matrix} [\nu_2] \\ L_2\beta_2[\mu_2] S_2 \end{matrix} \right)_{\omega_2^0} F(A-B) \right]^{L[\mu]S}_{IY} \\ &= \sum_{\nu\tau\beta} C^{[\tilde{\nu}]\tau,\beta[\mu]S}_{[\tilde{\nu}_1]\beta_1[\mu_1]S_1,[\tilde{\nu}_2]\beta_2[\mu_2]S_2} \left| \begin{matrix} [\nu] & \tau[\nu_1][\nu_2] \\ L\beta[\mu] IYS, & L_1\ L_2 \end{matrix} \right) . \end{aligned} \tag{9-24d}$$

9.4. Transformations between Symmetry Bases and Physical Bases in the Quark Model

Suppose A and B are two clusters consisting of f_1 and f_2 quarks, respectively. For clarity in our notation, we assume that there are only two kinds of flavor quarks, u and d. The extension to more kinds of flavor quarks is straightforward. A quark is said to be in the orbital state a (b) if it belongs to the cluster A(B). The wave functions for describing the clusters A and B are taken to be expressed in the irreducible basis classified according to the following group chain

$$\begin{array}{lccccccc} & SU_{24} & \supset & SU_2 & \times & SU_{12} & (\supset & SU_3 \times SU_4) \\ & & & \text{orbital} & & & & \text{color} \quad \text{spin–isospin} \\ \text{irrep label:} & [1^{f_i}] & & [\nu_i] & & [\tilde{\nu}_i] & & [\sigma_i] \quad [\mu_i] \end{array}$$

In terms of the CG coefficients of the permutation group, the aforesaid basis is expressed as

$$\left| \begin{matrix} [\nu_i] \\ [\sigma_i] W_i [\mu_i] S_i T_i \end{matrix} \right) = \sum_{m_1 m_2 m} \frac{\Lambda_m^{\nu_i}}{\sqrt{h_{\nu_i}}} C^{[\tilde{\nu}_i],\tilde{m}}_{\sigma_i m_1, \mu_i m_2} \psi_m^{[\nu_i]}(\mathbf{r}) \left| \begin{matrix} [\sigma_i] \\ m_1, W_i \end{matrix} \right\rangle \left| \begin{matrix} [\mu_i] \\ m_2, S_i T_i \end{matrix} \right\rangle , \tag{9-25a}$$

where $\psi(\mathbf{r})$ is the orbital wave function and W_i are the component indices for irreps of SU_3 in color space. For instance, a nucleon N and its resonance state Δ are described by [compare with (7-112b) and (7-112c)]

$$|N) = \left| \begin{matrix} [3] \\ [1^3][3]\frac{1}{2}, \frac{1}{2} \end{matrix} \right) , \quad |\Delta) = \left| \begin{matrix} [3] \\ [1^3][3]\frac{3}{2}, \frac{3}{2} \end{matrix} \right) . \tag{9-25b}$$

The totally anti-symmetric wave functions of these two clusters can be expressed by

$$\mathcal{A} \left[\left| \begin{matrix} [\nu_1] a^{f_1} \\ \sigma_1 \mu_1 S_1 T_1 \end{matrix} \right)_{\omega_0^1} \left| \begin{matrix} [\nu_2] b^{f_2} \\ \sigma_2 \mu_2 S_2 T_2 \end{matrix} \right)_{\omega_0^2} \right]^{[\sigma] S T}_{W M_S M_T} , \tag{9-26a}$$

where the square bracket indicates the couplings in terms of the SU_3 and SU_2 CG coefficients so that they have definite SU_3 symmetry $[\sigma]W$, definite channel spin S and isospin T. Equation (9-26a) has been referred to as the *physical basis* [Harvey (1981)], since it has a clear physical meaning. Nevertheless, in order to exploit the CFP technique in the evaluation of matrix elements, it is preferable to use the following $SU_{24} \supset SU_2 \times SU_{12} (\supset SU_3 \times SU_4)$ basis for the $n = f_1 + f_2$ quarks,

$$\left| \begin{matrix} [\nu] a^{f_1} b^{f_2} \\ \alpha [\sigma] W [\mu] \beta S T M_S M_T \end{matrix} \right) . \tag{9-26b}$$

Equation (9-26b) is referred to as the *symmetry basis*. In analogy with (9-23), the physical and symmetry bases differ by a unitary transformation

$$\begin{aligned} &\mathcal{A} \left[\left| \begin{matrix} [\nu_1] a^{f_1} \\ \sigma_1 \mu_1 S_1 T_1 \end{matrix} \right)_{\omega_0^1} \left| \begin{matrix} [\nu_2] b^{f_2} \\ \sigma_2 \mu_2 S_2 T_2 \end{matrix} \right)_{\omega_0^2} \right]^{[\sigma] S T} \\ &\quad = \sum_{\tilde{\nu} \alpha \mu \varphi \beta} C^{[\tilde{\nu}], \alpha [\sigma] [\mu] \varphi}_{\tilde{\nu} \sigma_1 \mu_1, \tilde{\nu}_2 \sigma_2 \mu_2} C^{[\mu] \varphi, \beta S T}_{\mu_1 S_1 T_1, \mu_2 S_2 T_2} \left| \begin{matrix} [\nu] a^{f_1} b^{f_2} \\ \alpha [\sigma] [\mu] \beta S T \end{matrix} \right) , \end{aligned} \tag{9-27a}$$

where the first factor on the right-hand side is the $SU_{12} \supset SU_3 \times SU_4$ ISF, and the second is the $SU_4 \supset SU_2 \times SU_2$ ISF.

Table 9.3. The transformation matrix between the physical and symmetry bases.

$S=1,T=1$	$\left\vert\begin{matrix}[51]\\ [2^3][42]\end{matrix}\right)$	$\left\vert\begin{matrix}[33]\\ [2^3][42]\end{matrix}\right)$	$\left\vert\begin{matrix}[33]\\ [2^3][6]\end{matrix}\right)$	$\left\vert\begin{matrix}[42]\\ [2^3][51]\end{matrix}\right)$	$\left\vert\begin{matrix}[42]\\ [2^3][411]\end{matrix}\right)$
$(\Delta\Delta)$	$-\sqrt{\frac{20}{45}}$	$-\sqrt{\frac{16}{45}}$	$\sqrt{\frac{9}{45}}$	0	0
$(N\Delta)_1$	$\sqrt{\frac{5}{45}}$	$\sqrt{\frac{4}{45}}$	$\sqrt{\frac{36}{45}}$	0	0
$(N\Delta)_2$	0	0	0	1	0
$(CC')_1$	$-\sqrt{\frac{4}{9}}$	$\sqrt{\frac{5}{9}}$	0	0	0
$(CC')_2$	0	0	0	0	-1

The symmetry basis can be expanded in terms of the $SU_{24} \supset SU_2 \times SU_{12}$ ($\supset SU_3 \times SU_4 (\supset SU_2 \times SU_2)$) CFP. Using the Racah factorization lemma and (7-244b), we can immediately write down

$$\left\vert \begin{matrix}[\nu]w\\ \alpha[\sigma][\mu]\beta ST\end{matrix}\right) = \sum \sqrt{\frac{h_{\nu'} h_{\nu''}}{h_\nu}} C^{[\tilde{\nu}],\alpha[\sigma][\mu]\varphi}_{\tilde{\nu}'\sigma'\mu',\tilde{\nu}''\sigma''\mu''} C^{[\sigma]w}_{\nu'w',\nu''w''} C^{[\mu]\varphi,\beta ST}_{\mu' S'T',\mu'' S''T''}$$
$$\times \left[\left\vert \begin{matrix}[\nu']w'\\ \sigma'\mu' S'T'\end{matrix}\right)_{1\ldots n_1} \left\vert \begin{matrix}[\nu'']w''\\ \sigma''\mu'' S''T''\end{matrix}\right)_{n_1+1\ldots n} \right]^{[\sigma]ST} , \tag{9-27b}$$

where the sum runs over $\sigma'\mu' w' S'T' \sigma''\mu'' w'' S''T''$ and φ. w', w'' and w are the Weyl tableaux resulting from filling the Young diagrams $[\nu']$, $[\nu'']$ and $[\nu]$, respectively, with the state indices a and b. $C^{[\nu]w}_{\nu'w',\nu''w''}$ is the SU_2 CG coefficient, or in other words the orbital CFP. It is clearly from the previous discussion that in such a calculation, the $SU_{mn} \supset SU_m \times SU_n$ ISF plays a crucial role.

Example: We calculate the transformation matrix between the physical and symmetry bases for the channel $S = T = 2$.

From (9-27a) and using the $SU(mn) \supset SU(m) \times SU(n)$ ISF table, Table IV–5–13a, 13e, 78b, 80i and 81i in Chen, Wu & Gao (1991) we can calculate the transformation matrix shown in Table 9.3.
where

$$(N\Delta)_i = \sqrt{\frac{1}{2}} \left[\mathcal{A}(|N)|\Delta)) - (-1)^i \mathcal{A}(|\Delta)|N)) \right] ,$$
$$(CC')_i = \sqrt{\frac{1}{2}} \left[\mathcal{A}(|C)|C')) - (-1)^i \mathcal{A}(|C')|C)) \right] ,$$
$$|C) = \left\vert \begin{matrix}[3]\\ [21][21]1/2, 3/2\end{matrix}\right) , \quad |C') = \left\vert \begin{matrix}[3]\\ [21][21]3/2, 1/2\end{matrix}\right) . \tag{9-27c}$$

(CC′) is the so-called hidden color channel, since the three-quark clusters C as well as C′ are not color singlets. Instead, they have the symmetry [21] in color space. However, the six-quark cluster is in the color singlet $[2^3]$. Table 9.3 agrees with Harvey's (1981) Table 11. For further discussion see Chen, Shi (1983).

9.5. The Dynamical Symmetry Models of Nuclei

The relatively simple structure of the spectra of low-lying nuclei prompted the development of phenomenological collective models. The simplicity in the spectra was interpreted as arising

from collective vibrations and rotations of the nuclei. Among these the most prominent and successful models are the Bohr–Mottelson (1953) geometric model and the Arima–Iachello (1976) interacting boson model (IBM).

The microscopic interpretation of such collective motion is a challenging problem. However great simplification occurs when the system has a *dynamical symmetry*, which means, as we have already mentioned in Sec. 3.20.3, that its Hamiltonian can be written in terms of the generators of a Lie algebra and is only a linear function of the Casimir operators of a complete chain of groups. For such cases the eigenvalue and eigenfunction of H can have analytic expressions. The first dynamical symmetry nuclear model was the Elliott model but it was the IBM which pushed the nuclear dynamic symmetry to the foreground and revived the interest of nuclear physicists in group theory. An important lesson one learns from these pioneering works is that each dynamical symmetry is associated with a particular collective mode.

In the following sections we shall introduce both the boson dynamic symmetry model, that is the IBM, and several fermion dynamical symmetry models (FDSM), which include the pairing and neutron-proton pairing models, and the Elliott model (Elliott 1958). From these exactly solvable models one can see clearly the power and elegance of group theory in its application to the many-body problem.

We will see that all these FDSM's have a common group structure. The dynamical group G involves particle number non-conserving operators, which consist of the raising operators and lowering operators. The group G contains a subgroup $G_1 \times G_2$, where G_1 is a particle number conserving group and is called the core group, while $G_2 = U_1 \sim SO_2$ has the particle number operator as its generator. In the cases discussed here the group chain $G \supset G_1 \times G_2$ has the form of $SO_n \supset SO_{n-2} \times SO_2$, with $n = 3, 5$. The vector coherent state theory (Rowe 1985, Hecht 1987) provides an elegant means for dealing with such algebras.

In the following we use $|\ \rangle$ and $|\ )$ to represent a boson and a fermion state, respectively.

9.6. The Quasispin Model

Let us consider n nucleons in a single j-shell and suppose that the short-range residual interaction is the predominant one. The interaction is approximated by the pairing force

$$H_{SU2} = -G_0 S^\dagger S \ , \tag{9-28}$$

$$S^\dagger = S_+ = \sqrt{\frac{\Omega}{2}}[C_j^\dagger C_j^\dagger]_0^0 = \sum_{m>0} s_+^{(m)} \ , \tag{9-29}$$

where $\Omega = j + \frac{1}{2}, S^\dagger$ is the creation operator for a pair of nucleons with $J = 0$, and

$$s_+^{(m)} = (-)^{j-m} C_m^\dagger C_{-m}^\dagger \ , \quad C_m^\dagger \equiv C_{jm}^\dagger \ . \tag{9-30a}$$

Introducing

$$s_0^{(m)} = \frac{1}{2}(\hat{n}_m + \hat{n}_{-m} - 1), \quad s_-^{(m)} = (s_+^{(m)})^\dagger \ . \tag{9-30b,c}$$

we have the commutator

$$[s_+^{(m)}, s_-^{(m)}] = 2s_0^{(m)}, \quad [s_0^{(m)}, s_\pm^{(m)}] = \pm s_\pm^{(m)} \ . \tag{9-30d}$$

Thus $(s_+^{(m)} s_-^{(m)}, s_0^{(m)})$ form the algebra su_2. From (9-30b) we see that

$$s_0^{(m)} = \begin{cases} 1/2 \\ -1/2 \\ 0 \end{cases} \quad \text{if} \quad \begin{cases} (m,-m) \text{ is full} \\ (m,-m) \text{ is empty} \\ (m,-m) \text{ is singly occupied} \ . \end{cases} \tag{9-31a}$$

Therefore one can associate each pair level $(m,-m)$ with a *quasispin* $\mathbf{s}^{(m)}$ (Kerman 1961, Eisenberg 1976),

$$\mathbf{s}^{(m)} = \begin{cases} 1/2 \\ 0 \end{cases} \quad \text{if} \begin{cases} (m,-m) \text{ is full or empty} \\ (m,-m) \text{ is singly occupied} . \end{cases} \tag{9-31b}$$

The total quasispin operators are denoted by S_+, S_-, S_0, where $S_- = (S_+)^\dagger$, and

$$S_0 = \sum_{m>0} s_0^{(m)} = \frac{1}{2}(\hat{n} - \Omega) , \quad \hat{n} = \sum_m C_m^\dagger C_m . \tag{9-32}$$

The commutators between S_+, S_-, and S_0 are identical with (9-30d). S_+, S_- and S_0 form the quasispin algebra su_2 . We can take over all the results from the angular momentum theory; for example, its irreps can be labelled by the quasispin S. The Chevalley basis for the quasispin SU_2 is,

$$E_\alpha = S_+ , \quad E_{-\alpha} = S_- , \quad H_\alpha = 2S_0 = \hat{n} - \Omega , \quad [E_\alpha, E_{-\alpha}] = H_\alpha . \tag{9-33}$$

The pairing Hamiltonian (9-28) can be expressed in terms of the Casimir operator $\mathbf{S}^2$ of the quasispin SU_2 group,

$$H_{SU_2} = -G_0[\mathbf{S}^2 - S_0(S_0 - 1)] . \tag{9-34}$$

Therefore the pairing Hamiltonian has the quasispin SU_2 as its dynamical group.

The particle number non-conserving Lie group SU_2 has the structure of $SO_3 \supset SO_1 \times SO_2$, the core group SO_1 is the trivial identity transformation group and the generator of SO_2 is $S_0 = (\hat{n} - \Omega)/2$. The irreducible basis of the core group SO_1 and the lowest weight (l.w.) state of SU_2 is denoted by $|v, \alpha JM\rangle$, where α represents extra quantum numbers other than JM for labeling the v-particle state with angular momentum JM. The quantum number v is called the *seniority* and is the number of nucleons entirely free of S pairs. This basis satisfies,

$$S_-|v, \alpha JM\rangle = 0 . \tag{9-35}$$

In the language of coherent state theory, the state $|v\alpha JM\rangle$ is called the intrinsic state. To avoid confusion with the intrinsic state defined by (3-151), we call it coherent intrinsic state. According to (9-32) the weight for the l.w. state is $(S_0)_{\min} = \frac{1}{2}(v - \Omega)$. Hence the highest weight is

$$S = -(S_0)_{\min} = \frac{1}{2}(\Omega - v) . \tag{9-36}$$

Relation (9-36) can be easily understood by noting that when all Ω pair levels are full or empty, S reaches its maximal value $\frac{\Omega}{2}$, a sum of Ω spin-$\frac{1}{2}$ entities. For a state with seniority v, v pair levels are singly occupied, and consequently only $(\Omega - v)$ pair levels contribute to the total quasispin and S is thus reduced to $\frac{1}{2}(\Omega - v)$.

It is more convenient to use the seniority v, which has direct physical meaning, instead of the quasispin S to label irreps of the quasispin SU_2. Similarly we use $n = v, v+2, v+4, \ldots, 2\Omega - v$, instead of $S_0 = -S, -S+1, \ldots, S$, as the component index of the irrep $v = \Omega - 2S$. By applying a power of the raising operator $S^\dagger$ to the coherent intrinsic state, we can obtain other states of the same irrep v, since $S^\dagger$ is the generator of SU_2 and thus does not change the irrep v. Therefore the eigenfunction of H_{SU_2} can be written as

$$|v, n\alpha JM\rangle = \eta_{nv}(S^\dagger)^{(n-v)/2}|v\alpha JM\rangle . \tag{9-37}$$

The following equation is very useful for evaluating the norm η_{nv}. Suppose that

$$[A, B] = X, \quad [[A, B], B] = Y, \quad [Y, B] = 0 . \tag{9-38}$$

We then have the identity

$$\begin{aligned}[A, B^n] &= \sum_{i=0}^{n-1} B^i X B^{n-i-1} \\ &= \sum_{i=0}^{n-1} \left[B^i \sum_{j=0}^{n-i-2} B^j Y B^{n-i-j-2} + B^{n-1} X \right] \\ &= \sum_{i=0}^{n-1} (n-i-1) B^{n-2} Y + n B^{n-1} X \\ &= \binom{n}{2} B^{n-2} Y + n B^{n-1} X \ . \end{aligned} \tag{9-39}$$

Using (9-30d), that is,

$$[S, S^\dagger] = -2S_0 = \Omega - \widehat{n} \ , \tag{9-40}$$

as well as (9-39) and $\widehat{n}|v\alpha JM\rangle = v|v\alpha JM\rangle$, we have

$$\begin{aligned}\eta_{nv}^{-2} &= \langle v\alpha JM | S^{(n-v)/2} (S^\dagger)^{(n-v)/2} | v\alpha JM \rangle \\ &= \left(\frac{n-v}{4} \right) (2\Omega - n - v + 2) \eta_{n-2,v}^{-2} \ . \end{aligned} \tag{9-41a}$$

By induction we obtain the norm

$$\eta_{nv} = \left[\frac{2^{n-\Omega} (2\Omega - n - v)!!}{(n-v)!! (\Omega - v)!} \right]^{1/2} \ . \tag{9-41b}$$

The eigenvalue of H_{SU2} is obtained from (9-34), (9-32) and (9-36),

$$E_{nv} = -\frac{G_0}{4} (n-v)(2\Omega - n - v + 2) \ . \tag{9-42}$$

Since $G_0 > 0$ for an attractive pairing force, we see that the state with lowest seniority, that is the state with as many as possible S pairs, lies lowest in energy. The highest weight state is

$$[v, n = 2\Omega - v, \alpha, JM\rangle = \frac{1}{(\Omega - v)!} (S^\dagger)^{\Omega - v} | v\alpha JM \rangle \ . \tag{9-43}$$

Notice that the vacuum state $|0\rangle$ belongs to the irrep with the highest quasispin $\Omega/2$ rather than the identity rep of SU_2.

9.7. The Proton–Neutron Quasispin Model

In the previous section we considered only one kind of nucleons. Now we introduce the proton–neutron quasispin model (Parikh 1965, Hecht 1985). The single particle creation operator is denoted by $C^\dagger_{mtz} \equiv C^\dagger_{jm,\frac{1}{2}tz}$, with $t_z = \frac{1}{2}$ for the proton and $t_z = -\frac{1}{2}$ for the neutron. The shell degeneracy is enlarged to $\Omega = 2j + 1$ and the pairing Hamiltonian is extended to

$$H_{SO_5} = -G_0 \mathcal{S}^\dagger \cdot \mathcal{S} \equiv -G_0 \sum_q \mathcal{S}_q^\dagger \mathcal{S}_q \ , \tag{9-44}$$

$$\mathcal{S}_q = \sqrt{\frac{\Omega}{2}} \left[C^\dagger_{j\frac{1}{2}} C^\dagger_{j\frac{1}{2}} \right]^{01}_{0q} \ . \tag{9-45}$$

The operator $\mathcal{S}_q^\dagger$ creates a pair of nucleons with $J=0$ and $T=1, T_z=q$. The total isospin operators are

$$T_\mu = \sqrt{\frac{\Omega}{2}}[C^\dagger_{j\frac{1}{2}}\tilde{C}_{j\frac{1}{2}}]^{01}_{0\mu}\ , \quad T_{\pm 1} = \mp\sqrt{\frac{1}{2}}T_\pm\ , \quad T_0 = T_z\ , \tag{9-46a}$$

$$\tilde{C}_{jm,\frac{1}{2}\mu} = (-)^{j+m+\frac{1}{2}+\mu}C_{j-m,\frac{1}{2}-\mu}\ . \tag{9-46b}$$

The following operators form the Cartan–Weyl basis for the quasispin group $SO_5 \sim Sp_4$,

$$\begin{aligned} &H_1 = \tfrac{1}{2}(\hat{n}-\Omega)\ , \quad H_2 = T_z = \tfrac{1}{2}(\hat{n}_1-\hat{n}_2)\ , \quad E_{01} = \tfrac{1}{\sqrt{2}}T_+\ , \\ &E_{11} = \tfrac{1}{\sqrt{2}}S^\dagger(1)\ , \quad E_{10} = \tfrac{1}{\sqrt{2}}S^\dagger(0)\ , \qquad E_{1-1} = \tfrac{1}{\sqrt{2}}S^\dagger(-1)\ . \end{aligned} \tag{9-47}$$

$$\begin{aligned} &E_{-i-k} = (E_{ik})^\dagger\ , \quad ik = 11, 10, 1-1, 01\ . \\ &\hat{n} = \hat{n}_1 + \hat{n}_2\ , \qquad \hat{n}_\mu = \sum_m C^\dagger_{m\mu}C_{m\mu}\ , \end{aligned} \tag{9-48}$$

where $\mu = \frac{1}{2}$ and $-\frac{1}{2}$ are indexed as 1 and 2 respectively. The Lie algebra has the structure $so_5 \supset so_3 \oplus so_2$ (or $sp_4 \supset su_2 \oplus u_1$). The core algebra is $su_2 \sim so_3 = (T_1, T_{-1}, T_z)$, while $so_2 = H_1$. The raising operators are $S_q^\dagger$. The commutator relations are

$$[H_1, H_2] = 0\ , \quad [H_1, E_{ik}] = iE_{ik}\ , \quad [H_2, E_{ik}] = kE_{ik}\ ,$$

$$[E_{ik}, E_{i'k'}] = \begin{cases} NE_{i+i',k+k'}, & \text{if } (i+i', k+k') \text{ is a root, } N = \pm 1\ , \\ 0, & \text{otherwise} \end{cases} \tag{9-49}$$

$$[E_{ik}, E_{-i-k}] = iH_1 + kH_2\ .$$

The simple roots are $(1,-1)$ and $(0,1)$ while the Chevalley basis is

$$\begin{array}{lll} E_{\alpha_i}: \tfrac{1}{2}A^\dagger_{22}, & & B_{12} \\ \qquad\quad \alpha_1 & \longrightarrow & \alpha_2 \\ H_{\alpha_i}: n_2 - \tfrac{1}{2}\Omega & & n_1 - n_2 \end{array}$$

Fig. 9.7. The Chevalley basis of SO_5.

where

$$A^\dagger_{\alpha\beta} = \sum_m (-)^{j-m}C^\dagger_{m\alpha}C^\dagger_{-m\beta}\ , \tag{9-50a}$$

$$B_{\alpha\beta} = \sum_m C^\dagger_{m\alpha}C_{m\beta} - \frac{\Omega}{2}\delta_{\alpha\beta}\ . \tag{9-50b}$$

We see that $E_{\alpha_1} = -E_{1-1}$ and $E_{\alpha_2} = \sqrt{2}E_{01}$. The eigenvalue of (H_1, H_2), denoted as $[L_1, L_2]$, is the *Cartan–Weyl label* of SO_5, while the eigenvalue (a_1, a_2) of $(H_{\alpha_1}, H_{\alpha_2})$ is the *Dynkin label* of SO_5. They are related by $L_1 = a_1 + a_2/2, L_2 = a_2/2$. The Casimir operator of SO_5 is

$$\begin{aligned} C_{SO_5} &= H_1^2 + H_2^2 + \sum_{\alpha>0}(E_\alpha E_{-\alpha} + E_{-\alpha}E_\alpha) \\ &= \sum_q \mathcal{S}_q^\dagger \mathcal{S}_q + \mathbf{T}^2 - H_1(-H_1+3)\ . \end{aligned} \tag{9-51a}$$

Using (9-47) and (9-51a) we have

$$H_{SO_5} = -G_0 \left[C_{SO_5} + \tfrac{1}{4}(\hat{n} - \Omega)(\Omega - \hat{n} + 6) - \mathbf{T}^2\right] . \tag{9-51b}$$

Therefore H_{SO_5} is a function of the Casimir operators of the group chain $SO_5 \supset SO_3$ and thus has a dynamical symmetry. The eigenvalue of C_{SO_5} can be found from (5-352f),

$$C_{SO_5} = L_1(L_1 + 3) + L_2(L_2 + 1) . \tag{9-51c}$$

Let $|\beta(v, \tau\tau_z), \alpha JM\rangle$ be states of v nucleons totally free of any $\mathcal{S}$ pairs,

$$\mathcal{S}_q|\beta(v, \tau\tau_z)\ , \alpha JM\rangle = 0\ , \quad \text{for } \tau_z = \tau, \ldots, -\tau\ , \quad \text{and} \quad q = 0, \pm 1\ . \tag{9-51d}$$

They are irreducible bases of the core group SU_2 with isospin τ, τ_z, and are called *vector coherent states*. The quantum numbers v and τ are the seniority and *reduced isospin*, respectively, while β is an additional quantum number used to specify the states uniquely.

Applying (H_1, H_2) to the state $|\beta(v, \tau, -\tau), \alpha JM\rangle$ we find the lowest weight $[\frac{v-\Omega}{2}, \tau]$ for the SO_5 irrep generated from the vector coherent states. The highest weight of SO_5 is

$$[L_1 L_2] = \left[\frac{\Omega - v}{2}, \tau\right] . \tag{9-51e}$$

Therefore we can use (v, τ) as the irrep label for SO_5. A general irreducible basis can be constructed (Hecht 1985) by acting $p = (n - v)/2$ pair creation operators with the resultant isospin T_p on the vector coherent states, and by coupling τ and T_p to the total isospin T in terms of the SU_2 CG coefficients

$$|n, \beta(v, \tau) T_p T M_T, \alpha JM\rangle = \left[P_{pT_p}(\mathcal{S}^\dagger)|\beta(v, \tau), \alpha JM\rangle\right]^T_{M_T} . \tag{9-52a}$$

$P_{pT_pM_p}(\mathcal{S}^\dagger)$ is called the raising polynomial and is a product of p pair creation operators $\mathcal{S}^\dagger_q$ coupled to $T_p = p, p-2, \ldots, 0$ or 1,

$$P_{pT_pM_p}(\mathcal{S}^\dagger) = \mathcal{N}_{pT}(\mathcal{S}^\dagger \cdot \mathcal{S})^{(p-T_p)/2} \mathbf{Y}_{T_pM_p}(\mathcal{S}^\dagger) , \tag{9-52b}$$

$$\mathcal{N}_{pT} = \left[\frac{4\pi(p + T_p)!!}{(p - T_p)!!(p + T_p + 1)!}\right]^{1/2} , \tag{9-52c}$$

where $\mathbf{Y}_{T_pM_p}(\mathcal{S}^\dagger)$ is the solid spherical harmonics $[\mathbf{Y}_{LM}(\mathbf{r}) = r^L Y_{LM}(\theta\varphi)]$. Notice that the states (9-52a) are not normalized, and if several T_p are possible for fixed n, τ and T, then the states with different T_p have a non-zero overlap. The problem of constructing orthonormalized wave functions is solved satisfactorily by the vector coherent state theory (Rowe 1985, Hecht 1987).

It will be shown that (9-52a) is the irreducible basis vector for the group chain $U_{2\Omega} \supset (U_\Omega \supset Sp_\Omega \supset SO_3) \times SU_2$.

The eigenvalue of H_{SO_5} in the state (9-52a) is obtained from (9-51b), (9-47) and (9-51e),

$$E_{nvt} = -G_0 \left[\frac{1}{4}(n - v)(2\Omega - n - v + 6) + \tau(\tau + 1) - T(T + 1)\right] . \tag{9-52d}$$

It is seen that the state with low seniority and low isospin T lies low in energy.

For identical nucleons, $T = \frac{n}{2}, \tau = \frac{v}{2}$, (9-52d) reduces to (9-42) with G_0 replaced by $2G_0$.

9.8. The Groups Sp_N, SO_N and the Pairing Interaction

In Sections 9.6 and 9.7 we used the quasispin group, the particle–number non–conservation group, to treat the pairing interaction. In this section we are going to show that the same problem can be handled by using the Sp_N or SO_N group. This approach was adopted in Racah (1943, 1949) and in Edmonds & Flowers (1952), using first quantization. It has the advantage that it reveals the close relationship between the pairing and symplectic or orthogonal group. We will treat the same problem by using the second quantization, which is simpler than the first quantization.

9.8.1. Pairing interaction for identical particles

As in Sec. 5.9 we use a to denote the angular momentum of single particle states, and a can be integer $a = l$ or half–integer $a = j$. The group G_N with $N = 2a + 1$ is the group SO_N and Sp_N for $a = l$ and j respectively.

The pairing interaction Q was introduced by Racah (1943) in the first quantization formalism,

$$Q = \sum_{i<j} q_{ij} \ , \quad \langle a^2 JM | q_{ij} | a^2 JM \rangle = (2a+1)\delta_{J0} \ . \tag{9-53a}$$

In the second quantization,

$$Q = \mathcal{S}^\dagger \mathcal{S} = \frac{1}{2} \sum_{\alpha,\beta} C^\dagger_\alpha C^\dagger_{\tilde{\alpha}} C_{\tilde{\beta}} C_\beta \ , \quad \mathcal{S}^\dagger = \sqrt{\frac{2a+1}{2}} (C^\dagger_a C^\dagger_a)^0_0 \ , \tag{9-53b}$$

where $\mathcal{S}^\dagger$ is defined as in (5-166a) and is related to the quasispin operator $S^\dagger$ in (9-29) by $\mathcal{S}^\dagger = \sqrt{2} S^\dagger$. The operator $C^\dagger_\alpha \equiv C^\dagger_{a\alpha}$ is a boson (fermion) operator for $a = l(j)$. Our goal is to find the relation between the pairing interaction Q and the Casimir operator of G_N.

Using (5-163d) we have

$$P^r \cdot P^r = \sum_J (2r+1) W(aaaa; rJ) (C^\dagger_a C^\dagger_a)^J \cdot (\tilde{C}_a \tilde{C}_a)^J + \frac{2r+1}{2a+1} \hat{n} \ , \tag{9-54a}$$

$$2\mathcal{S}^\dagger \mathcal{S} = \sum_r (-1)^r P^r \cdot P^r - (-1)^{2a} \hat{n} \ . \tag{9-54b}$$

From (9-54a) we know that when acting on a single particle state, $C^\dagger_{a\alpha}|0\rangle$, $P^r \cdot P^r = \frac{2r+1}{2a+1}$. Therefore $p^r \cdot p^r$ is a constant,

$$p^r \cdot p^r = \frac{2r+1}{2a+1} \ . \tag{9-54c}$$

From (5-222) and (9-54b) we obtain an important relation between the Casimir operators of U_N, G_N and the pairing Hamiltonian,

$$C_{G_{2a+1}} = C_{U_{2a+1}} - (-1)^{2a} \hat{n} - 2\mathcal{S}^\dagger \mathcal{S} \ . \tag{9-54d}$$

This shows that the pairing Hamiltonian is a linear function of the Casimir operators of the groups U_{2a+1} and G_{2a+1}, namely it has dynamical symmetry.

Since $C^\dagger_{a\alpha}$ is a boson or fermion operator, the Casimir operator of U_N for identical particles can be reduced to

$$C_{U_N} = \sum_{\alpha\beta} C^\dagger_\alpha C_\beta C^\dagger_\beta C_\alpha = \hat{n} N + (-1)^{2a} \hat{n}(\hat{n}-1) = \begin{cases} \hat{n}(N + \hat{n} - 1), & a = l \\ \hat{n}(N - \hat{n} + 1), & a = j \end{cases} \ . \tag{9-55a}$$

Notice that the same formula can be obtained from (5-355a) by letting $[\nu] = [n]$ and $[\nu] = [1^n]$ for $a = l$ and $a = j$, respectively.

From (9-54d) and (9-55a) we have

$$C_{Sp_N} = C_{U_N} + n - 2\mathcal{S}^\dagger\mathcal{S} = n(N+2-n) - 2\mathcal{S}^\dagger\mathcal{S} \ . \tag{9-55b}$$

Applying (9-55b) to the state $|v, \alpha JM\rangle$ defined in (9-35) we get the eigenvalue of the Casimir operator of Sp_N

$$C_{Sp_N}(v) = v(N+2-v) \ . \tag{9-55c}$$

From (9-55b,c) we obtain the the pairing energy as a function of n and the seniority v,

$$Q(nv)|_{Sp_N} = \mathcal{S}^\dagger\mathcal{S} = \frac{1}{2}[n(N+2-n) - v(N+2-v)] = \frac{n-v}{2}(N+2-n-v) \ , \tag{9-56a}$$

which is just (9-42) (Noting that $\mathcal{S}^\dagger\mathcal{S} = 2S^\dagger S$).

Similarly, from (9-54d) and (9-55a), we have

$$C_{SO_N} = C_{U_N} - n - 2\mathcal{S}^\dagger\mathcal{S} = n(N-2+n) - 2\mathcal{S}^\dagger\mathcal{S}. \tag{9-56b}$$

Let $|v\alpha LM\rangle$ be a state of v bosons free of $\mathcal{S}$ pairs. The eigenvalue of the Casimir operator of SO_N is

$$C_{SO_N}(v) = v(N-2+v). \tag{9-56c}$$

From (9-56b,c) we obtain the the pairing energy for n bosons,

$$Q(nv)|_{SO_N} = \mathcal{S}^\dagger\mathcal{S} = \frac{n-v}{2}(N-2+n+v) \ . \tag{9-56d}$$

It is interesting to compare (9-56a) and (9-56d). For given v the quantum number n takes

$$n = \begin{cases} v, v+2, \ldots, N-v, & \text{for } Sp_N \ , \\ v, v+2, \ldots, & \text{for } SO_N \ . \end{cases} \tag{9-56e}$$

Thus the maximum number of paired fermions is $N - v = 2j + 1 - v$, due to the Pauli principle, while there is no restriction on the number of paired boson. If the pairing interaction between bosons is attractive, the ground state is the one which has as many as possible paired bosons and thus gives rise to boson condensation.

9.8.2. Pairing interaction for electrons and non-identical nucleons

Let us consider the following pairing interaction

$$Q = \frac{1}{2}\sum_{\alpha\beta,\mu\mu'} C^\dagger_{\alpha\mu} C^\dagger_{\tilde{\alpha}\mu'} C_{\tilde{\beta}\mu'} C_{\beta\mu} = \sum_q \mathcal{S}^\dagger_q \mathcal{S}_q \ , \tag{9-57a}$$

$$\mathcal{S}^\dagger_q = \sqrt{\frac{2a+1}{2}} \left[C^\dagger_{a\frac{1}{2}} C^\dagger_{a\frac{1}{2}}\right]^{01}_{0q} \ , \tag{9-57b}$$

where $C^\dagger_{\alpha,\mu} \equiv C^\dagger_{a\alpha,\xi\mu}$, $a = l, j$ for electron and nucleon, $\xi = \frac{1}{2}$ is spin and isospin for electron and nucleons, respectively, and $C^\dagger_{\tilde{\alpha}\mu'} = (-1)^{a+\alpha} C^\dagger_{-\alpha\mu'}$.

The eigenvalue of the Casimir operator of U_N is given in (5-352f,g) as a function of partitions. By letting $[\nu] = [2^{\frac{n}{2}-S}1^{2S}]$ or $[\nu] = [2^{\frac{n}{2}-T}1^{2T}]$ into (3-352), we can get the eigenvalue as a function of the spin S or isospin T. Replacing the eigenvalues $S(S+1)$ and $T(T+1)$ by the corresponding operators, we get the operator identity

$$C_{U_N} = \begin{cases} \frac{\hat{n}}{2}(2N+4-\hat{n}) - 2\mathbf{S}\cdot\mathbf{S} & \text{for electrons} \ , \\ \frac{\hat{n}}{2}(2N+4-\hat{n}) - 2\mathbf{T}\cdot\mathbf{T} & \text{for nucleons} \ , \end{cases} \tag{9-57c}$$

where the Casimir operator C_{U_N} is given in (5-222a) with P^r interpreted as $\mathbf{P}^r$ of (5-161c); the spin and isospin operators are obtained from Eq. (5-161b) and the reduced matrix elements $\langle \frac{1}{2} \| s \| \frac{1}{2} \rangle_{\mathrm{Ed}} = \langle \frac{1}{2} \| t \| \frac{1}{2} \rangle_{\mathrm{Ed}} = \sqrt{\frac{3}{2}}$,

$$S_\mu = \sqrt{\frac{2l+1}{2}} \left[C^\dagger_{l\frac{1}{2}} \tilde{C}_{l\frac{1}{2}} \right]^{01}_{0\mu}, \quad T_\mu = \sqrt{\frac{2j+1}{2}} \left[C^\dagger_{j\frac{1}{2}} \tilde{C}_{j\frac{1}{2}} \right]^{01}_{0\mu}. \tag{9-57d}$$

Equation (9-54d) remains valid under the replacement $\mathcal{S}^\dagger \mathcal{S} \to \sum_q \mathcal{S}^\dagger_q \mathcal{S}_q$. From (9-54d) and (9-57c) we obtain the Casimir operators of G_N,

$$C_{SO_N} = \frac{\hat{n}}{2}(2N + 2 - \hat{n}) - 2\mathbf{S} \cdot \mathbf{S} - 2\sum_q \mathcal{S}^\dagger_q \mathcal{S}_q \,, \tag{9-57e}$$

$$C_{Sp_N} = \frac{\hat{n}}{2}(2N + 6 - \hat{n}) - 2\mathbf{T} \cdot \mathbf{T} - 2\sum_q \mathcal{S}^\dagger_q \mathcal{S}_q \,. \tag{9-57f}$$

Using (9-57e) we find the eigenvalue of C_{SO_N}, in a state with v electrons free of any $\mathcal{S}$ pairs and with total spin S, to be

$$C_{SO_N}(vS) = \frac{v}{2}(2N + 2 - v) - 2S(S+1) \,. \tag{9-58a}$$

Similarly, according to (9-57f), the eigenvalue of C_{Sp_N} in a state with v nucleons free of any $\mathcal{S}$ pairs and with total isospin τ is

$$C_{Sp_N}(v\tau) = \frac{v}{2}(2N + 6 - v) - 2\tau(\tau+1) \,. \tag{9-58b}$$

From (9-57e) and (9-58a) we have the pairing energy for n electrons with seniority v

$$Q(nv)|_{SO_N} = \frac{1}{4}(n - v)(2N + 2 - n - v) \,. \tag{9-58c}$$

Eq. (9-58c) was first obtained by Racah (1942), who used first quantization methods to obtain it.

Similarly for the Sp_N case from (9-57f) and (9-58b) we obtain the pairing energy in a state with n nucleons, seniority v, reduced isospin τ and total isospin T,

$$Q(nv\tau T)|_{Sp_N} = \mathcal{S}^\dagger \mathcal{S} = \frac{1}{4}(n - v)(2N - n - v + 6) + \tau(\tau+1) - T(T+1) \,, \tag{9-58d}$$

which is just (9-52d). For identical nucleons with $T = \frac{n}{2}$ and $\tau = \frac{v}{2}$, Eq. (9-58b) and (9-58d) reduce to (9-55c) and (9-56a), respectively.

From (9-51a), (9-57f) and (9-47) (which reads $H_1 = \frac{1}{2}(n - N)$), we obtain

$$2C_{SO_5} + C_{Sp_N} = \tfrac{1}{2}N(N+6) \,. \tag{9-58e}$$

Therefore the $SO_5 \supset SU_2 \times U_1$ irreducible basis (9-52) is also the irreducible basis for the group chain $U_{2N} \supset (U_N \supset Sp_N \supset SO_3) \times SU_2$. To make things more clear, we need to trace back to the largest group involved in this case. For a system with n nucleons in the single-particle state j with isospin $\frac{1}{2}$, there are 2^{2N} states, which carry the basic representation [1] of the group $U_{2^{2N}}$ (Wybourne 1974). Two group chains are available for classifying the states. These two group chains and the corresponding quantum numbers for the groups are (Sun 1993):

$$\begin{array}{llllcllll} U_{2^{2N}} \supset & O_{4N} \supset & [Sp_N \supset & SO_3] & \otimes & [SO_5 \supset & SU_2 & \times & U_1] \\ [1] & [\sigma] & (v\tau) & \alpha J & & (v\tau) & \beta T & & h_1 \end{array} \tag{9-58f}$$

and

$$\begin{array}{cccccccc} U_{2^{2N}} \supset & O_{4N} \supset & SU_{2N} \supset & [SU_N \supset & Sp_N \supset & SO_3] & \otimes & SU_2 \\ [1] & [\sigma] & [1^n] & [\tilde{\nu}_T] & \beta(v\tau) & \alpha J & & T \end{array} \tag{9-58g}$$

where $[\sigma] = [(\frac{1}{2})^{2N}]$ and $[(\frac{1}{2})^{2N-1} - \frac{1}{2}]$ for even and odd number of nucleons, respectively, and $[\tilde{\nu}_T]$ is the conjugate of $[\nu_T] = [\frac{n}{2} - T, 2T]$. The quantum numbers β and α in (9-58g) are multiplicity labels for the subduction $SU_N \downarrow Sp_N$ and $Sp_N \downarrow SO_3$, respectively.

From (9-58e) we know that the states (9-52) are irreducible basis vectors for both the group chains (9-58f) and (9-58g). This enables us to derive simple relations between the $U_N \supset Sp_N$ ISF and the $SO_5 \supset SU_2 \times U_1$ ISF so that the former can be calculated from the latter (Sun 1993).

Notice an essential difference between (9-58c) and (9-58d): the pairing is independent of the total spin S for the former while it depends on the total isospin T in the latter. The reason is that the $\mathcal{S}$ pair in the SO_N case has $L = 0, S = 0$, while in the Sp_N case, $J = 0$ and $T = 1$. The state vector for n electrons with total orbital angular momentum L, total spin S and seniority v can be constructed as

$$|n\alpha LMSM_S\rangle = \text{const } (\mathcal{S}^\dagger)^{\frac{n-v}{2}} |v\alpha LMSM_S\rangle \ , \tag{9-58h}$$

which is to be compared with the corresponding equation (9-52a).

Finally, let us look at the relation between the quantum number $(vS)((v\tau))$ and the partitions $[\sigma]$, the Cartan–Weyl label, of the orthogonal (symplectic) groups. Suppose that a system of v electrons which is free of $\mathcal{S}$ pairs has the permutational symmetry

$$[\sigma_1\sigma_2 \ldots \sigma_a] = [2^{\frac{v}{2}-S}1^{2S}] \ . \tag{9-59a}$$

Then the eigenvalue of C_{SO_N} in this state can be calculated using (5-352f)

$$C_{SO_N}(vS) = \sum_i \sigma_i(\sigma_i + N - 2i) = \frac{v}{2}(2N + 2 - v) - 2S(S+1) \ . \tag{9-59b}$$

This is just (9-58a). Thus the irreps of SO_N can be labelled in this case by either the partition $[\sigma] = [2^{\frac{v}{2}-S}1^{2S}]$ or the quantum numbers v, S.

Similarly suppose that a state of v nucleons which is free of any $\mathcal{S}$ pairs has the permutational symmetry

$$[\sigma_1\sigma_2 \ldots \sigma_{a+1/2}] = [2^{\frac{v}{2}-\tau}1^{2\tau}] \ . \tag{9-59c}$$

The eigenvalue of C_{Sp_N} in this state can be calculated using (5-352g),

$$C_{Sp_N}(v\tau) = \sum_i \sigma_i(\sigma_i + 2 + N - 2i) = \frac{v}{2}(2N + 6 - v) - 2\tau(\tau + 1) \ . \tag{9-59d}$$

This is just (9-58b).

9.9. The Elliott Model

We now consider the other extreme case where the long-range force predominates. In the Elliott model, nucleons are assumed to move in an isotropic harmonic potential with the residual interaction simulated by the following separable force, called quadrupole–quadrupole (Q–Q) force

$$H_{SU_3} = -B_2 \sum_\mu (-)^\mu P^2_\mu P^2_{-\mu} = -B_2 P^2 \cdot P^2 \ , \tag{9-60a}$$

$$P^2_\mu = \sum_{j=1}^n q^{(j)}_\mu \ , \tag{9-60b}$$

$$q_\mu = \sqrt{\frac{\pi}{10}} i^2 [r^2 Y_{2\mu}(\mathbf{r}) + p^2 Y_{2\mu}(\mathbf{p})] = -\sqrt{\frac{1}{8}} q_\mu(\text{Elliott}) \ . \tag{9-60c}$$

Within a single major shell, the operator q_μ is equivalent to

$$q_\mu = \sqrt{\frac{2\pi}{5}} r^2 i^2 Y_{2\mu}(\theta, \varphi) \ . \tag{9-60d}$$

Notice that we use $i^l Y_{l\mu}$ instead of $Y_{l\mu}$ as the basis function, and that in (9-60a) we included the one–body term $\sum_j q^{(j)} \cdot q^{(j)}$.

The Hamiltonian of the Elliott model is

$$H = H_0 + H_{SU_3} \ , \ H_0 = \sum_{j=1}^{n} \left[\frac{\mathbf{p}_j^2}{2m} + \frac{k}{2} \mathbf{r}_j^2 \right] .$$

We define the dipole operator P^1_μ by

$$P^1_\mu = \sqrt{\tfrac{3}{8}} L_\mu = \sqrt{\tfrac{3}{8}} \sum_{j=1}^{n} (\mathbf{r}_j \times \mathbf{p}_j) \ . \tag{9-60e}$$

It is convenient to shift to the second quantized form. Eq. (5-159a) can be extended to

$$P^r_\mu = \sum_{LL'} \sqrt{\frac{2L+1}{2r+1}} \langle L \| P^r \| L' \rangle (b^\dagger_L \tilde{b}_{L'})^r_\mu \ . \tag{9-61}$$

Using the oscillator wave functions, the reduced matrix elements of P^r_μ can be calculated and (9-61) can be written down explicitly (Elliott 1958),

$$P^1_\mu = \sum_L \sqrt{\frac{L(L+1)(2L+1)}{8}} (b^\dagger_L \tilde{b}_L)^1_\mu \ , \tag{9-62a}$$

$$P^2_\mu = \frac{1}{\sqrt{8}} \sum_L \left[(2N+3) \sqrt{\frac{L(L+1)(2L+1)}{5(2L-1)(2L+3)}} (b^\dagger_L \tilde{b}_L)^2_\mu \right.$$
$$\left. + \sqrt{\frac{6(L+1)(L+2)(N-L)(N+L+3)}{5(2L+3)}} (b^\dagger_L \tilde{b}_{L+2} + b^\dagger_{L+2} \tilde{b}_L)^2_\mu \right] . \tag{9-62b}$$

It should be mentioned that since we use $i^l Y_{l\mu}$ as basis, the sign of the first term is opposite to that given by Elliott.

For the $1p$ shell, $N = 1, L = 1$ and the quanta $b^\dagger_{1m}$ is denoted by $c^\dagger_m$. The harmonic oscillator potential has SU_3 as a symmetry group, whose defining basis is $c^\dagger_m|0\rangle, m = 1, -1$ and 0, which are indexed as $i = 1, 2$ and 3, respectively. The states $m = 1, -1$ (or $i = 1, 2$) form the defining basis for an SU_2 symmetry, whose irreducible basis is labelled by the "spin" Λ and its third component Λ_z. Letting $N = 1, L = 1$ in (9-62) we can obtain P^r_μ in terms of $c^\dagger_m c_{m'}$, which can be put in the following unified form,

$$P^r_\mu = \frac{\sqrt{3}}{2} \sum_{mm'} (-)^{1+m'} C^{r\mu}_{1m,1m'} E_{m,-m'}, \quad r = 1, 2 \ . \tag{9-63}$$

$$E_{mm'} = c^\dagger_m c_{m'} \equiv B_{mm'} - \frac{1}{2} \delta_{mm'} \ . \tag{9-64}$$

The nine operators $E_{mm'}, m, m' = 1, -1, 0$ are the generators of U_3. The commutators for P^r_μ are obtainable from (5-163a)

$$[P^r, P^s]^t_\sigma = \frac{\sqrt{3}}{2} (-)^t [1 - (-)^{r+s+t}] \widehat{rs} \begin{Bmatrix} r & s & t \\ 1 & 1 & 1 \end{Bmatrix} P^t_\sigma \ , \quad t = 1, 2 \ , \tag{9-65}$$

Equation (9-65) describes the commutators for the Lie algebra su_3. The weight operators are

$$H_1 = -\sqrt{8}P_0^2 = 2n_0 - n_1 - n_{-1}\ , \quad H_2 = L_Z = n_1 - n_{-1}\ . \tag{9-66}$$

The eigenvalue of H_1 is denoted by ε which describes the magnitude of the quadrupole deformation of a nucleus, and $H_2/2$ is equal to Λ_z.

In the s–d shell, $N = 2, L = 0$ and 2. From (9-62) we then have

$$\mathcal{P}_\mu^2 = (d^\dagger \tilde{s} + s^\dagger \tilde{d})_\mu^2 + \frac{\sqrt{7}}{2}(d^\dagger \tilde{d})_\mu^2\ , \tag{9-67a}$$

$$\mathcal{P}_\mu^1 = \frac{\sqrt{15}}{2}(d^\dagger \tilde{d})_\mu^1\ , \tag{9-67b}$$

where we write $d_m^\dagger = b_{2m}^\dagger, s^\dagger = b_{00}^\dagger$. The commutators of $\mathcal{P}_\mu^r$ can be evaluated using (5-163),

$$[\mathcal{P}^1, \mathcal{P}^1]_\sigma^t = \frac{\sqrt{3}}{2}\delta_{t1}\mathcal{P}_\sigma^1\ , \quad [\mathcal{P}^2\ , \mathcal{P}^2]_\sigma^t = \frac{\sqrt{15}}{2}\delta_{t1}\mathcal{P}_\sigma^1\ , \tag{9-68a}$$

$$[\mathcal{P}^1, \mathcal{P}^2]_\sigma^t = \sqrt{6}\delta_{t2}\mathcal{P}_\sigma^2\ . \tag{9-68b}$$

Note that the commutators (9-65) and (9-68) are the same in spite of their different appearances.

The two-quanta creation operator $b_{LM}^\dagger$ with $L = 0, 2$ can be expressed as

$$b_{LM}^\dagger = \sum_{mm'} C_{1m,1m'}^{LM} A_{mm'}^\dagger\ , \quad A_{mm'}^\dagger = c_m^\dagger c_{m'}^\dagger\ . \tag{9-69}$$

Therefore $d^\dagger$ and $s^\dagger$ can be thought of as " compound particles", and $c_m^\dagger$ can be regarded as the "Elliott quark". $s^\dagger$ and $d^\dagger$ form the $SU_3 \supset SO_3$ basis belonging to the SU_3 irrep (20). On the other hand, the $A_{mm'}^\dagger$ form the $SU_3 \supset SU_2$ basis of the same irrep (20) of SU_3. From (9-69) we have,

$$d_2^\dagger = A_{11}^+\ , \quad d_1^\dagger = \sqrt{2}A_{13}^\dagger\ , \quad d_0^\dagger = \sqrt{\tfrac{2}{3}}(A_{12}^\dagger + A_{33}^\dagger)\ , \tag{9-70a}$$

$$d_{-2}^\dagger = A_{22}^\dagger\ , \quad d_{-1}^\dagger = \sqrt{2}A_{23}^\dagger\ , \quad s^\dagger = \tfrac{1}{\sqrt{3}}(2A_{12}^\dagger - A_{33}^\dagger)\ , \tag{9-70b}$$

$$\sqrt{2}A_{12}^\dagger = \tfrac{1}{\sqrt{3}}(\sqrt{2}s^\dagger + d_0^\dagger)\ , \quad A_{33}^\dagger = \tfrac{1}{\sqrt{3}}(\sqrt{2}d_0^\dagger - s^\dagger)\ . \tag{9-70c}$$

The Casimir operator of SU_3 is

$$C_{SU_3} = \sum_{r=1}^{2} P^r \cdot P^r\ . \tag{9-71a}$$

Its eigenvalue is obtained from (5-304c) and (9-63),

$$C_{SU_3}(\lambda\mu) = (\lambda^2 + \mu^2 + \lambda\mu + 3\lambda + 3\mu)/2\ . \tag{9-71b}$$

H_{SU_3} can be written in terms of the Casimir operators of the group chain $SU_3 \supset SO_3$,

$$H_{SU_3} = -B_2\Big[C_{SU_3} - \tfrac{3}{8}L(L+1)\Big]\ . \tag{9-72a}$$

The Elliott model exploits the symmetries and degeneracies of the harmonic-oscillator Hamiltonian and has found useful applications in the nuclei at the beginning of the s–d shell, $16 < A < 24$. In the s–d shell, there are six orbital states and four spin–isospin states. The totally anti-symmetric state is adapted to the following group chain,

$$\begin{array}{ccccccc} SU_{24} & \supset & (SU_6 & \supset & SU_3 & \supset & SO_3) \times SU_4 \\ [1^n] & & [f] & & (\lambda\mu) & & KLM \quad [\tilde{f}] \end{array} \tag{9-72b}$$

where $[f]$ is a partition of the number of nucleons in the s–d shell, $\lambda = 2h_1 - 2h_2, \mu = 2h_2 - 2h_3, [2h_1, 2h_2, 2h_3]$ is the partition of the total quanta number $2n$, and K is the third component of $\mathbf{L}$ in the intrinsic coordinate system (Sec. 6.7). The $SU_6 \downarrow SU_3$ and $SU_3 \downarrow SO_3$ subduction rules are given in Elliott (1958). The orbital wave function is denoted by $|[f](\lambda\mu)KLM)$. Using (9-72a) we have,

$$H_{SU_3}|[f](\lambda\mu)KLM) = E_L^{(\lambda\mu)}|[f](\lambda\mu)KLM) \tag{9-72c}$$

$$E_L^{(\lambda\mu)} = -\frac{B_2}{2}\left[C_{SU_3}(\lambda\mu) - \frac{3}{8}L(L+1)\right] . \tag{9-72d}$$

The significance of the Elliott model is that for the first time it gave a microscopic description of nuclear collective rotations, and revealed the important fact that the dynamical SU_3 symmetry is associated with the rotational mode.

Similar to Moshinsky (1968), we can find the $SU_3 \supset SU_2 \times U_1$ basis for a given irrep $(\lambda\mu)$ from its highest weight state |h.w.),

$$|(\lambda\mu)\varepsilon\Lambda K) = \left|\begin{pmatrix} 2h_1\, 2h_2\, 2h_3 \\ h_{12}\, h_{22} \\ h_{11} \end{pmatrix}\right\rangle$$

$$= N_{h_{11}}^{h_{12}h_{22}} N_{h_{12}h_{22}}^{h_1h_2h_3} (B_{21})^{h_{12}-h_{11}} (B_{13})^{h_{12}-2h_2} (L_{23})^{h_{22}-2h_3} |\text{h.w.}) , \tag{9-73a}$$

where B_{ij} are defined in (9-64), the relations between the quantum numbers $(\lambda\mu), \varepsilon, \Lambda$ and K on the one hand, and the entries of the Gel'fand symbol on the other, are

$$\lambda = 2h_1 - 2h_2 , \quad \mu = 2h_2 - 2h_3 , \quad \varepsilon = 8n - 3(h_{12} + h_{22}) , \tag{9-73b}$$

$$\Lambda = (h_{12} - h_{22})/2 , \qquad K = 2h_{11} - (h_{12} + h_{22}) , \tag{9-73c}$$

while the other quantities in (9-73a) are

$$L_{23} = B_{23}(B_{11} - B_{22} + 1) - B_{21}B_{13} , \tag{9-73d}$$

$$N_{h_{11}}^{h_{12}h_{22}} / N_{h_{11}-1}^{h_{12}h_{22}} = [(h_{12} - h_{11} + 1)(h_{11} - h_{22})]^{1/2} , \tag{9-74a}$$

$$N_{h_{12}h_{22}}^{h_1h_2h_3} / N_{h_{12}-1h_{22}}^{h_1h_2h_3} = \left[\frac{(h_{12} - h_{22} + 1)}{(h_{12} - 2h_2)(h_{12} - 2h_3 + 1)(2h_1 - h_{12} + 1)}\right]^{1/2} , \tag{9-74b}$$

$$N_{h_{12}h_{22}-1}^{h_1h_2h_3} / N_{h_{12}h_{22}}^{h_1h_2h_3} = [(h_{12} - h_{22} + 2)(2h_1 - h_{22} + 2)(2h_2 - h_{22} + 1)(h_{22} - 2h_3)]^{1/2} . \tag{9-74c}$$

The highest weight state |h.w.) can be constructed with the same technique used by Castanos (1984) for the $Sp(6,R) \supset U_3$ wave functions. The result is

$$|\text{h.w.}) = |(\lambda\mu)\varepsilon_h\Lambda_hK_h) = \left|\begin{pmatrix} 2h_1\, 2h_2\, 2h_3 \\ 2h_2\, 2h_3 \\ 2h_2 \end{pmatrix}\right\rangle$$

$$= N_{h_1h_2h_3}(A_{33}^\dagger)^{h_1-h_2}(\Delta_{22}^\dagger)^{h_2-h_3}(\Delta^\dagger)^{h_3}|0) , \tag{9-75a}$$

where $\varepsilon_h = 2\lambda + \mu, \Lambda_h = \frac{\mu}{2}, K_h = \mu$, and

$$\Delta^\dagger = \begin{vmatrix} A_{11}^\dagger & A_{12}^\dagger & A_{13}^\dagger \\ A_{12}^\dagger & A_{22}^\dagger & A_{23}^\dagger \\ A_{13}^\dagger & A_{23}^\dagger & A_{33}^\dagger \end{vmatrix} , \tag{9-75b}$$

$$N_{h_1h_2h_3} = \left[\frac{h_2!2^{h_2-h_1-h_3}(h_1-h_3+1)!(2h_1-2h_2+1)!!(2h_2-2h_3+1)!!}{(h_1+1)!(h_1-h_2)!(h_2-h_3)!h_3!(2h_2+1)!(2h_1-2h_3+1)!!}\right]^{1/2}, \qquad (9\text{-}75c)$$

with $\Delta^\dagger_{ij}$ the cofactor of the determinant $\Delta^\dagger = (= \Sigma_{ij} A^\dagger_{ij}\Delta^\dagger_{ij})$.

The $SU_3 \supset SU_2 \times U_1$ state is referred to as the intrinsic state, which is precisely the intrinsic state $\Phi_0^{(K)}(X)$ discussed in Sec. 6.6 and 6.7. Using (6-70) we can project out the physical basis with good angular momentum from the intrinsic state.

Since the Q–Q force is attractive, (9-72d) and (9-71b) show that the larger the deformation $\varepsilon_h = 2\lambda + \mu$, the larger the eigenvalue $C_{SU_3}(\lambda\mu)$, and the lower the energy of the state.

9.10. The Interacting Boson Model*

Although the Elliott model is elegant, it's direct applicability to heavier nuclei is made impractical by the strong spin–orbit force, which pushes down the level $j = l + 1/2$ of the unique parity in the N–th shell down to the $(N-1)$–th shell. However most of the rotational nuclei are medium–heavy and heavy nuclei. Arima and Iachello introduced the interacting boson model (IBM) and greatly extended the application region of the Elliott model. By re–interpreting the quanta creation operators $s^\dagger$ and $d^\dagger$ in the Elliott model as the creation operators of s and d bosons which are the approximations of the coherent fermion pairs with $J = 0$ and 2, respectively, we are led to the IBM. In the IBM, an even–even nuclei with n valence nucleons is approximated as a N–boson system, $N = n/2$, interacting through one– and two–body forces. Each boson has two possible states, either $L = 0$, corresponding to an s boson, or $L = 2$, corresponding to a d boson, and they span the defining rep of the group SU_6. The IBM Hamiltonian can be conveniently expressed in terms of the boson multipole operators P^r_μ,

$$H_B = \varepsilon_s N_s + \varepsilon_d N_d + B_0 C_{U_5} + \sum_{r=1}^{3} B_r P^r(\chi_r)\cdot P^r(\chi_r)\ , \qquad (9\text{-}76a)$$

$$P^r_\mu(\chi_r) = \delta_{r2}(d^\dagger\tilde{s} + s^\dagger\tilde{d})^2_\mu + (-)^{[(r-1)/2]}\chi_r(d^\dagger\tilde{d})^r_\mu, \quad r = 1,2,3\ , \qquad (9\text{-}76b)$$

where N_s and N_d are the numbers of s and d bosons, $N = N_s + N_d$ is the total number of bosons, and C_{U_5} is the Casimir operator of U_5 (9-55a),

$$C_{U_5} = N_d(N_d+4)\ . \qquad (9\text{-}77)$$

The group U_6 has three subgroup chains containing the rotation group SO_3,

$$\begin{array}{rl} & \nearrow\ U_5 \ \rightarrow SO_5 \rightarrow SO_3 \\ U_6 \rightarrow & SO_6 \rightarrow SO_5 \rightarrow SO_3\ . \\ & \searrow\ SU_3 \rightarrow SO_3 \end{array} \qquad (9\text{-}78a)$$

Using the method described in Sec. 5.24.3, we can find the Chevalley basis for the various subgroups in (9-78a) as well as bases for the basic and identity reps of these subgroups. The results are listed in Tables 9.10 and Figs. 9.10, where

$$\mathcal{B}_{ij} = b^\dagger_i b_j\ , \quad N_i = b^\dagger_i b_i \qquad (9\text{-}78b)$$

and the indexing of the boson operators for each case are given in Table 9.10-1b, -2b and -3b.

Table 9.10-1a. The Chevalley basis of SO_5.

	$\mathcal{B}_{12}+\mathcal{B}_{45}$	$\sqrt{2}(\mathcal{B}_{23}+\mathcal{B}_{34})$	$\mathcal{B}_{14}+\mathcal{B}_{25}$	$\sqrt{2}(\mathcal{B}_{13}-\mathcal{B}_{35})$
$H_{\alpha_1} = N_1 - N_2 + N_4 - N_5$	2	−1	0	1
$H_{\alpha_2} = 2(N_2 - N_4)$	−2	2	2	0

Table 9.10-1b. Bases of the basic and identity reps of SO_5.

	$d_2^\dagger$ $b_1^\dagger$	$d_1^\dagger$ $b_2^\dagger$	$d_0^\dagger$ $b_3^\dagger$	$d_{-1}^\dagger$ $b_4^\dagger$	$d_2^\dagger$ $b_5^\dagger$	$s^\dagger$ $b_6^\dagger$	$d^\dagger \cdot d^\dagger$
$H_{\alpha_1} = N_1 - N_2 + N_4 - N_5$	1	−1	0	1	−1	0	0
$H_{\alpha_2} = 2(N_2 - N_4)$	0	2	0	−2	0	0	0

Table 9.10-2a. The Chevalley basis and roots of SO_6.*

	$\mathcal{B}_{26} + \mathcal{B}_{34}$	$\mathcal{B}_{12} + \mathcal{B}_{45}$	$\mathcal{B}_{23} + \mathcal{B}_{64}$	$\mathcal{B}_{16} - \mathcal{B}_{35}$	$\mathcal{B}_{14} + \mathcal{B}_{25}$	$\mathcal{B}_{13} - \mathcal{B}_{65}$
$H_{\alpha_1} = q + l$	2	−1	0	1	1	−1
$H_{\alpha_2} = p - q$	−1	2	−1	1	0	1
$H_{\alpha_3} = q - l$	0	−1	2	−1	1	1

*$p = N_1 - N_5$, $q = N_2 - N_4$, $l = N_3 - N_6$.

Table 9.10-2b. Bases of the basic and identity reps of SO_6.

	$d_2^\dagger$ $b_1^\dagger$	$d_1^\dagger$ $b_2^\dagger$	$\sqrt{\frac{1}{2}}(d_0^\dagger + s^\dagger)$ $b_3^\dagger$	$d_{-1}^\dagger$ $b_4^\dagger$	$d_{-2}^\dagger$ $b_5^\dagger$	$\sqrt{\frac{1}{2}}(d_0^\dagger - s^\dagger)$ $b_6^\dagger$	$d^\dagger \cdot d^\dagger - s^\dagger \cdot s^\dagger$
$H_{\alpha_1} = N_2 + N_3 - N_4 - N_6$	0	1	1	−1	0	−1	0
$H_{\alpha_1} = N_1 - N_2 + N_4 - N_5$	1	−1	0	1	−1	0	0
$H_{\alpha_3} = N_2 - N_3 - N_4 + N_6$	0	1	−1	−1	0	1	0

Table 9.10-3a. The Chevalley basis and roots of SU_3.

	$\sqrt{2}(\mathcal{B}_{12} + \mathcal{B}_{23}) + \mathcal{B}_{64}$	$\sqrt{2}(\mathcal{B}_{34} + \mathcal{B}_{45}) + \mathcal{B}_{26}$	$\sqrt{2}(\mathcal{B}_{16} + \mathcal{B}_{65}) + \mathcal{B}_{24}$
$H_{\alpha_1} = 2(N_1 - N_3) + N_6 - N_4$	2	−1	1
$H_{\alpha_2} = 2(N_3 - N_5) + N_2 - N_6$	−1	2	1

Table 9.10-3b. Basis of the irrep (20) of SU_3.*

$(\varepsilon \Lambda K)$	$(-2\,1\,2)$	$(1\,\frac{1}{2}\,1)$	(400)	$(1\,\frac{1}{2}\,-1)$	$(-21-2)$	(-210)
	$A_{11}^\dagger$ $d_2^\dagger$ $b_1^\dagger$	$\sqrt{2}A_{13}^\dagger$ $d_1^\dagger$ $b_2^\dagger$	$A_{33}^\dagger$ $\sqrt{\frac{1}{3}}(\sqrt{2}\, d_0^\dagger - s^\dagger)$ $b_3^\dagger$	$\sqrt{2}A_{23}^\dagger$ $d_{-1}^\dagger$ $b_4^\dagger$	$A_{22}^\dagger$ $d_{-2}^\dagger$ $b_5^\dagger$	$\sqrt{2}A_{12}^\dagger$ $\sqrt{\frac{1}{3}}(d_0^\dagger + \sqrt{2}s^\dagger)$ $b_6^\dagger$
$H_{\alpha_1} = 2(N_1 - N_3) + N_6 - N_4$	2	0	−2	−1	0	1
$H_{\alpha_2} = 2(N_3 - N_5) + N_2 - N_6$	0	1	2	0	−2	−1

*The $A_{ij}^\dagger$ are defined by (9-70).

The elements associated with the simple roots in the Chevalley basis can be vividly seen in the following Dynkin diagrams:

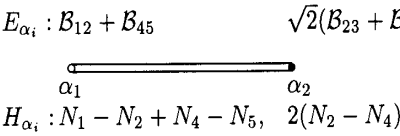


Fig. 9.10-1. The Chevalley basis of SO_5.

$$E_{\alpha_i}: \ \mathcal{B}_{26}+\mathcal{B}_{34},\ \mathcal{B}_{12}+\mathcal{B}_{45},\ \mathcal{B}_{23}+\mathcal{B}_{64}$$

$$H_{\alpha_i}: \quad q+l \qquad p-q \qquad q-l$$

Fig. 9.10-2. The Chevalley basis of SO_6.
$p = N_1 - N_5,\ q = N_2 - N_4,\ l = N_3 - N_6$

$$E_{\alpha_i}: \ \sqrt{2}(\mathcal{B}_{12}+\mathcal{B}_{23})+\mathcal{B}_{64}, \quad \sqrt{2}(\mathcal{B}_{34}+\mathcal{B}_{45})+\mathcal{B}_{26}$$

$$H_{\alpha_i}: 2(N_1-N_3)+N_6-N_4,\ 2(N_3-N_5)+N_2-N_6$$

Fig. 9.10-3. The Chevalley basis of SU_3.

The irreps of SO_5, SO_6, and SU_3 are labelled by the Dynkin labels $(\tau_1\tau_2), (\sigma_1\sigma_2\sigma_3)$ and $(\lambda\mu)$ respectively, which are the eigenvalues of $\{H_{\alpha_i}\}$ of the corresponding groups. From Tables 9.10 we see that in the (s,d) boson space, $\tau_2 = \sigma_1 = \sigma_3 = 0$, and both λ and μ are even. Therefore the irreps of SO_5 and SO_6 in the IBM are simply labelled by $\tau = \tau_1$ and $\sigma = \sigma_2$.

When the strength parameters take some special values, the Hamiltonian (9-76a) has a dynamical symmetry.

A. U_5 limit:

When $B_2 = 0$, the Hamiltonian (9-76a) becomes

$$H_{U_5} = \varepsilon_s N_s + \varepsilon_d N_d + B_0 C_{U_5} + \sum_{r=1,3} B_r P^r(\chi_r)\cdot P^r(\chi_r)\ . \tag{9-79}$$

By keeping $B_r\chi_r$ invariant, χ_r can be chosen freely without affecting the result. Let $\chi_1 = \chi_3 = \sqrt{2}$

$$\wp^r_\mu \equiv P^r_\mu(\sqrt{2}) = (-)^{[(r-1)/2]}\sqrt{2}(d^\dagger\tilde{d})^r_\mu, \quad r = 1,3\ . \tag{9-80a}$$

$$\wp^1_\mu = \sqrt{1/5}L_\mu\ . \tag{9-80b}$$

The ten operators $\wp^r_\mu, r = 1,3$, form the Lie algebra so_5 with the commutators

$$[\wp^r,\wp^s]^t_\sigma = -\sqrt{2}[1-(-)^{r+s+t}]\ \hat{r}\,\hat{s}(-)^{[t/2]}\begin{Bmatrix} r & s & t \\ 2 & 2 & 2 \end{Bmatrix}\wp^t_\sigma\ . \tag{9-81}$$

For computing boson commutators the following formulas are useful

$$[b_i, f(b_i^\dagger, b_i)] = \frac{\partial}{\partial b_i^\dagger} f(b_i^\dagger, b_i)\ , \tag{9-82a}$$

$$[b_i^\dagger, f(b_i^\dagger, b_i)] = -\frac{\partial}{\partial b_i} f(b_i^\dagger, b_i)\ , \tag{9-82b}$$

where $f(b_i^\dagger, b_i)$ is a function of the boson operators $b_i^\dagger$ and b_i. The Casimir operator of SO_5 is

$$C_{SO_5} = \sum_{r=1,3} \wp^r\cdot\wp^r\ . \tag{9-83}$$

Therefore H_{U_5} can be re-written as

$$H_{U_5} = \varepsilon_s N_s + \varepsilon_d N_d + B_0 C_{U_5} + B_3 C_{SO_5} + \frac{1}{5}(B_1 - B_3)\mathbf{L}^2\ . \tag{9-84a}$$

This has the dynamical symmetry $U_5 \supset SO_5 \supset SO_3$ and its eigenvalue is

$$E_{U_5} = \varepsilon_s N_s + \varepsilon_d N_d + B_0 N_d(N_d+4) + B_3\tau(\tau+3) + \frac{1}{5}(B_1 - B_3)L(L+1) , \tag{9-84b}$$

which resembles the spectra of an anharmonic vibrator.

According to Table 9.10-1b, $(d_2^\dagger)^\tau|0)$ is the highest weight state of the SO_5 irrep $(\tau,0)$. Therefore

$$|\tau; JM) = |\tau; 2\tau, 2\tau) = \frac{1}{\sqrt{\tau!}}(d_2^\dagger)^\tau|0) . \tag{9-85}$$

The basis function for the irrep τ of SO_5 with JM other than $(2\tau,2\tau)$ can be obtained by operating a definite function of $\wp^1$ and $\wp^3$ on (9-85),

$$\begin{aligned} &|\tau n_\Delta JM) = f_{n_\Delta JM}(\wp^1, \wp^3)|\tau, 2\tau, 2\tau) \\ &\equiv (d_\mu^\dagger)^\tau_{n_\Delta JM}|0) = \sum_{\sum t_\mu = \tau} C^{n_\Delta JM}_{t_2 \ldots t_{-2}} (d_2^\dagger)^{t_2} \ldots (d_{-2}^\dagger)^{t_{-2}}|0) , \end{aligned} \tag{9-86}$$

where n_Δ is an additional quantum number which counts the number of triplets of d bosons coupled to $J=0$. Obviously we have

$$(d \cdot d)(d_2^\dagger)^\tau|0) = 0 . \tag{9-87}$$

Since $(d \cdot d)$ is an invariant of SO_5, that is, $[\wp_\mu^\tau, (d \cdot d)] = 0$, from (9-86) and (9-87) we have

$$(d \cdot d)|\tau n_\Delta JM) = 0 . \tag{9-88}$$

Therefore the quantum number τ has the physical meaning that it counts the number of d bosons not coupled to $J=0$, and is termed as the SO_5 *seniority* .

The general eigenfunctions for H_{U_5} is (Cf. (9-58h))

$$|NN_d\tau n_\Delta JM) = \eta_{NN_d\tau}(s^\dagger)^{(N-N_d)}(d^\dagger \cdot d^\dagger)^{(N_d-\tau)/2}|\tau n_\Delta JM) , \tag{9-89a}$$

$$\eta_{NN_d\tau} = \left[\frac{(2\tau+3)!!}{(N-N_d)!(N_d+\tau+3)!!(N_d-\tau)!!}\right]^{1/2} . \tag{9-89b}$$

The allowed values of N_d, τ and J are

$$\begin{aligned} &N_d = 0, 1, \ldots, N, \ \tau = N_d, N_d-2, \ldots 0 \quad \text{or} \quad 1 , \\ &\tau = 3n_\Delta + \lambda, \qquad n_\Delta = 0, 1, 2, \ldots \\ &J = \lambda, \lambda+1, \ldots, 2\lambda-2, 2\lambda . \end{aligned} \tag{9-90}$$

B. The O_6 limit:

The condition for the O_6 limit to occur is

$$\varepsilon_s = \varepsilon_d, \quad \chi_2 = B_0 = 0 .$$

Besides (9-80) and (9-81), the Lie algebra so_6 has the following extra generators and commutators

$$\wp_\mu^2 = P_\mu^2(0) = (d^\dagger \tilde{s} + s^\dagger \tilde{d})_\mu^2 , \quad \wp_0^2 = b_3^\dagger b_3 - b_6^\dagger b_6 , \tag{9-91}$$

$$[\wp^2, \wp^2]_\sigma^t = \sqrt{2}(-)^{[t/2]}\wp_\sigma^t, \ t = 1, 3 , \tag{9-92a}$$

$$[\wp^3, \wp^2]_\sigma^t = \sqrt{\frac{14}{5}}\delta_{t2}\wp_\sigma^2 , \quad [\wp_0^2, d_0^\dagger \pm s^\dagger] = \pm(d_0^\dagger \pm s^\dagger) . \tag{9-92b}$$

$$H_{SO6} = \varepsilon_s N + B_2 C_{SO6} + (B_3 - B_2) C_{SO_5} + \frac{1}{5}(B_1 - B_3)\mathbf{L}^2 \ , \tag{9-93a}$$

$$C_{SO6} = \sum_{r=1}^{3} \wp^r \cdot \wp^r \ , \tag{9-94}$$

$$E_{SO6} = \varepsilon_s N + B_2 \sigma(\sigma+4) + (B_3 - B_2)\tau(\tau+3) + \frac{1}{5}(B_1 - B_3)L(L+1) \ . \tag{9-93b}$$

The spectra given by (9-93b) corresponds to the γ unstable rotor.

From Table 9.10-2b we see that the state $(d_2^\dagger)^\tau|0)$ also belongs to the irrep $(0\tau 0)$ of SO_6, or the irrep $\sigma = \tau$. The invariant

$$\Im^\dagger = (d^\dagger \cdot d^\dagger - s^\dagger \cdot s^\dagger) \tag{9-95a}$$

of SO_6 is called a generalized pair. Clearly

$$(d \cdot d - s \cdot s)(d_2^\dagger)^\tau|0) = 0 \ . \tag{9-95b}$$

Thus $\sigma(=\tau)$ is the number of bosons totally free of the generalized pairs, and it is called the SO_6 *seniority* . The state for $\sigma > \tau$ is constructed as follows;

$$|N = \sigma, \sigma\tau, n_\Delta JM) = f_{\sigma\tau}(s^\dagger, \Im^\dagger)|\tau n_\Delta JM) \ , \tag{9-96a}$$

where $f_{\sigma\tau}(s^\dagger, \Im^\dagger)$ is a polynomial of $s^\dagger$ and $d_\mu^\dagger$ of order $(\sigma - \tau) = 0, 1, 2, \ldots$, and

$$f_{\sigma\tau}(s^\dagger, \Im^\dagger) = \sum_{p=0} D_p(\sigma\tau)(s^\dagger)^{\sigma-\tau-2p}(\Im^\dagger)^p, \quad f_{\sigma\sigma}(s^\dagger, \Im^\dagger) = 1 \ , \tag{9-96b}$$

and the coefficients $D_p(\sigma\tau)$ are determined by the requirement that there are no generalized pairs in $|\sigma\sigma\tau n_\Delta JM)$,

$$\Im|\sigma\sigma\tau n_\Delta JM) = 0 \ . \tag{9-97}$$

Using the commutators

$$[\Im, \Im^\dagger] = 4(3 + \hat{N}) \ , \quad [[\Im, \Im^\dagger], \Im^\dagger] = 8\Im^\dagger \ , \quad [\Im, s^\dagger] = 2s \ , \tag{9-98}$$

from (9-97) one obtains (Ginocchio 1980) a recursive formula for the $D_p(\sigma\tau)$,

$$D_{p+1}(\sigma\tau) = \frac{(\sigma - \tau - 2p)(\sigma - \tau - 2p - 1)}{4(p+1)(\sigma - p + 1)} D_p(\sigma\tau) \ . \tag{9-99a}$$

By induction and insertion of the value of $D_0(\sigma\tau)$, which is obtained from the normalization condition, we find the final expression for $D_p(\sigma\tau)$ to be

$$D_p(\sigma\tau) = \left[\frac{2^{\sigma+1}(\sigma-\tau)!(2\tau+3)!!}{(\sigma+1)!(\sigma+\tau+3)!}\right]^{1/2} \frac{(\sigma+1-p)!}{4^p(\sigma-\tau-2p)!p!} \ . \tag{9-99b}$$

Finally the state with $N > \sigma$ is given by

$$|N\sigma\tau n_\Delta JM) = \xi_{N\sigma}(\Im^\dagger)^{(N-\sigma)/2}|\sigma\sigma\tau n_\Delta JM) \ , \tag{9-100}$$

where

$$\xi_{N\sigma} = \left[\frac{(2\sigma+4)!!}{(N+\sigma+4)!!(N-\sigma)!!}\right]^{1/2} \ . \tag{9-101}$$

The ranges of the quantum numbers are well known,

$$\sigma = N, N-2, \ldots, 0 \text{ or } 1 ,$$
$$\tau = \sigma, \sigma-1, \ldots, 0 . \tag{9-102}$$

C. The U_3 limit:

The condition $\varepsilon_s = \varepsilon_d, B_3 = 0$ and $\chi_2 = -\frac{\sqrt{7}}{2}$ leads to the following boson Hamiltonian,

$$H_{SU_3} = \varepsilon_s N + \sum_{r=1,2} B_r \mathcal{P}^r \cdot \mathcal{P}^r , \tag{9-103a}$$

$$\mathcal{P}^1_\mu = \sqrt{\tfrac{3}{8}} L_\mu = P^1_\mu \left(\tfrac{\sqrt{15}}{2}\right), \quad \mathcal{P}^2_\mu = P^2_\mu \left(-\tfrac{\sqrt{7}}{2}\right) , \tag{9-103b}$$

where $\mathcal{P}^1_\mu$ and $\mathcal{P}^2_\mu$ are precisely the operators given by (9-67) in the Elliott model. Using (9-71a), (9-103a) can be re–written as

$$H_{SU_3} = \varepsilon_s N + B_2 C_{SU_3} + \tfrac{3}{8}(B_1 - B_2)\mathbf{L}^2 , \tag{9-103c}$$
$$E_{SU_3} = \varepsilon_s N + B_2 C_{SU_3}(\lambda\mu) + \tfrac{3}{8}(B_1 - B_2) L(L+1) . \tag{9-103d}$$

The weight operators are $\widehat{\varepsilon} = -\sqrt{8}P^2_0$ and $K = L_z$. The boson operators $s^\dagger$ and $d^\dagger_0$ are not the eigenoperators of $\widehat{\varepsilon}$. They can be recombined into $b^\dagger_3$ and $b^\dagger_6$ which are eigenoperators of $\widehat{\varepsilon}$,

$$b^\dagger_3 = \tfrac{1}{\sqrt{3}}(\sqrt{2}d^\dagger_0 - s^\dagger) , \quad b^\dagger_6 = \tfrac{1}{\sqrt{3}}(\sqrt{2}s^\dagger + d^\dagger_0) . \tag{9-104a}$$

The weight operators $\widehat{\varepsilon}$ and K can now be expressed as

$$\widehat{\varepsilon} = -\sum_\mu (-)^\mu |\mu| \widehat{N}_\mu + 4\widehat{N}_3 - 2\widehat{N}_6 , \quad K = \sum_\mu \mu \widehat{N}_\mu , \tag{9-104b}$$

where $\widehat{N}_\mu = d^\dagger_\mu d_\mu$, for $\mu = \pm 1, \pm 2$, and $\widehat{N}_i = b^\dagger_i b_i$, for $i = 3, 6$.

The IBM SU_3 wave function can be obtained from the SU_3 wave function in the Elliott model, (9-73)–(9-75), simply by interpreting the s, d quanta as the s, d bosons and replacing the SU_3 lowering operators $E_{ij} = c^\dagger_i c_j$ by $\mathcal{E}_{ij}$ which are obtained from Table 9.10-3a as

$$\mathcal{E}_{21} = \sqrt{2}(\mathcal{B}_{61} + \mathcal{B}_{56}) + \mathcal{B}_{42} = \sqrt{2}(b^\dagger_6 d_2 + d^\dagger_{-2} b_6) + d^\dagger_{-1} d_1 ,$$
$$\mathcal{E}_{23} = \sqrt{2}(\mathcal{B}_{54} + \mathcal{B}_{43}) + \mathcal{B}_{62} = \sqrt{2}(d^\dagger_{-2} d_{-1} + d^\dagger_{-1} b_3) + b^\dagger_6 d_1 , \tag{9-104c}$$
$$\mathcal{E}_{13} = \sqrt{2}(\mathcal{B}_{12} + \mathcal{B}_{23}) + \mathcal{B}_{64} = \sqrt{2}(d^\dagger_2 d_1 + d^\dagger_1 b_3) + b^\dagger_6 d_{-1} .$$

According to (9-70) and (9-104a), the determinant $\Delta^\dagger$ in (9-75b) can be written in terms of the boson operators as

$$\Delta^\dagger = \begin{vmatrix} d^\dagger_2 & \frac{1}{\sqrt{2}} b^\dagger_6 & \frac{1}{\sqrt{2}} d^\dagger_1 \\ \frac{1}{\sqrt{2}} b^\dagger_6 & d^\dagger_{-2} & \frac{1}{\sqrt{2}} d^\dagger_{-1} \\ \frac{1}{\sqrt{2}} d^\dagger_1 & \frac{1}{\sqrt{2}} d^\dagger_{-1} & b^\dagger_3 \end{vmatrix} . \tag{9-104d}$$

9.11 The Molecular Shell Model

In Secs. 9.1 and 9.2 the nuclear shell model was treated using Racah's CFP technique. The same technique can also be applied to the molecular shell model (Tang 1966, 1975). A new method was proposed by Paldus (1974, 1976) for the molecular shell model in which the many-electron wave functions are expressed in terms of the Gel'fand bases and the Hamiltonian is diagonalized directly without using the CFP. The most attractive feature of this new approach

is that it can easily be translated into a computer program and therefore makes a large–scale configuration–mixing calculation feasible.

9.11.1 The Hamiltonian as a function of infinitesimal operators of the unitary group

Moshinky (1962) pointed out that any one–body or two–body operator can be expressed in terms of the infinitesimal operators of the unitary group. In a second quantized representation, a one–body operator reads

$$F = \sum_{\alpha\beta} \langle \alpha | F | \beta \rangle E_{\alpha\beta} \ , \quad E_{\alpha\beta} = a_\alpha^\dagger a_\beta \ , \tag{9-105}$$

where $a_\alpha^\dagger (a_\beta)$ are creation (annihilation) operators, while α and β are labels of the single particle states.

A two–body operator V in second quantized representation may be written as

$$\begin{aligned} V &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \ , \\ \langle \alpha\beta | V | \gamma\delta \rangle &= \int \varphi_\alpha^*(1) \varphi_\beta^*(2) V_{12} \varphi_\gamma(1) \varphi_\delta(2) d\tau_1 d\tau_2 \ . \end{aligned} \tag{9-106}$$

For fermions we have

$$a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma = -a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta = E_{\alpha\gamma} E_{\beta\delta} - \delta_{\gamma\beta} E_{\alpha\delta} \ ,$$

while for bosons we have

$$a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma = a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta = E_{\alpha\gamma} E_{\beta\delta} - \delta_{\gamma\beta} E_{\alpha\delta} \ .$$

Therefore, regardless of fermions or bosons, we have

$$V = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle E_{\alpha\gamma} E_{\beta\delta} - \frac{1}{2} \sum_{\alpha\beta\delta} \langle \alpha\beta | V | \beta\delta \rangle E_{\alpha\delta} \ . \tag{9-107}$$

9.11.2 Spin-free approximation

Since "spin–free' is a good approximation in quantum chemistry (Matsen, 1974), it is convenient to separate the many–electron wave functions into two parts, one related to spin space, and the other to orbital space. An f-electron[1)] anti–symmetric wave function with definite spin (SM_S) and point group symmetry $(\lambda)\mu$ [hereafter referred to as *many–electron SALC* wave function] can be expressed as

$$\Psi(\beta\lambda\mu, SM_S) = \sum_m \frac{\Lambda_m^\nu}{\sqrt{h_\nu}} \Big| m, \begin{matrix}[\nu] \\ \beta\lambda\mu \end{matrix} \Big\rangle \Big| \begin{matrix}[\tilde{\nu}] \\ \tilde{m}, \ SM_s \end{matrix} \Big\rangle \ , \tag{9-108}$$

$$[\nu] = \left[2^{\frac{f}{2}-S}, 1^{2S} \right] \ , \quad [\tilde{\nu}] = \left[\tfrac{f}{2} + S, \ \tfrac{f}{2} - S \right] \ . \tag{9-109}$$

where $[\nu]$ labels the irrep of the group SU_n and the permutation group S_f, m is the Yamanouchi number and β contains any additional quantum numbers. Under the spin–free approximation we have

$$\langle \Psi(\beta\lambda\mu, SM_S) | H | \Psi(\beta'\lambda'\mu', S'M_s') \rangle = \delta_{\lambda\lambda'} \delta_{\mu\mu'} \delta_{SS'} \delta_{M_S M_S'} \left\langle \begin{matrix}[\nu] \\ \beta\lambda \end{matrix} \Big| H \Big| \begin{matrix}[\nu] \\ \beta'\lambda \end{matrix} \right\rangle \ , \tag{9-110}$$

$$\left\langle \begin{matrix}[\nu] \\ \beta\lambda \end{matrix} \Big| H \Big| \begin{matrix}[\nu] \\ \beta'\lambda \end{matrix} \right\rangle = \left\langle m, \begin{matrix}[\nu] \\ \beta\lambda\mu \end{matrix} \Big| H \Big| m, \begin{matrix}[\nu] \\ \beta'\lambda\mu \end{matrix} \right\rangle \ . \tag{9-111}$$

[1)] As a first approximation, f is taken as the number of valence electrons.

On the right-hand side of (9-110), only the matrix element in orbital space is left and its value is independent of m and μ. The spin S manifests itself only through the partition $[\nu]$ [see (9-109)].

Suppose that under a given circumstance there are n one-particle levels needed to be accounted for and which span the basic rep of the group U_n. Since the Gel'fand bases of the group U_n, $\left|\begin{smallmatrix}[\nu]\\ W\end{smallmatrix}\right\rangle$, form a complete set, the f-electron wave function $\left|\begin{smallmatrix}[\nu]\\ \beta\lambda\mu\end{smallmatrix}\right\rangle$ can be expanded as follows:

$$\left|\begin{smallmatrix}[\nu]\\ \beta\lambda\mu\end{smallmatrix}\right\rangle = \sum_{W} \left\langle \begin{smallmatrix}[\nu]\\ W\end{smallmatrix} \middle| \begin{smallmatrix}[\nu]\\ \beta\lambda\mu\end{smallmatrix} \right\rangle \left|\begin{smallmatrix}[\nu]\\ W\end{smallmatrix}\right\rangle . \tag{9-112}$$

Substituting this into (9-111), we get

$$\left\langle \begin{smallmatrix}[\nu]\\ \beta\lambda\end{smallmatrix} \middle| H \middle| \begin{smallmatrix}[\nu]\\ \beta'\lambda\end{smallmatrix} \right\rangle = \sum_{WW'} \left\langle \begin{smallmatrix}[\nu]\\ W'\end{smallmatrix} \middle| \begin{smallmatrix}[\nu]\\ W'\end{smallmatrix} \middle| \begin{smallmatrix}[\nu]\\ \beta'\lambda\mu\end{smallmatrix} \right\rangle \left\langle \begin{smallmatrix}[\nu]\\ \beta\lambda\mu\end{smallmatrix} \middle| \begin{smallmatrix}[\nu]\\ W\end{smallmatrix} \right\rangle \left\langle \begin{smallmatrix}[\nu]\\ W\end{smallmatrix} \middle| H \middle| \begin{smallmatrix}[\nu]\\ W'\end{smallmatrix} \right\rangle . \tag{9-113}$$

Here μ can take any permissible value. The problem of calculating the matrix elements of the spin-free approximation Hamiltonian, $\left\langle \begin{smallmatrix}[\nu]\\ W\end{smallmatrix} \middle| H \middle| \begin{smallmatrix}[\nu]\\ W'\end{smallmatrix} \right\rangle$ has been solved algebraically by Li and Paldus (1990, 1993). The remaining tasks are: (i) to find an appropriate subgroup chain of U_n which can provide additional quantum number β so that the irreducible bases $\left|\begin{smallmatrix}[\nu]\\ \beta\lambda\mu\end{smallmatrix}\right\rangle$ can be uniquely specified; (ii) to find the transformation coefficients $\left\langle \begin{smallmatrix}[\nu]\\ W\end{smallmatrix} \middle| \begin{smallmatrix}[\nu]\\ \beta\lambda\mu\end{smallmatrix} \right\rangle$ from the point group symmetry adapted irreducible basis $\left|\begin{smallmatrix}[\nu]\\ \beta\lambda\mu\end{smallmatrix}\right\rangle$ to the Gel'fand basis. These two problems have been solved satisfactorily (Gao 1987), but will not be presented here due to space limitations.

The unitary group approach turned out to be particularly useful in molecular electronic structure calculations, where only two-column irreducible representations need to be considered (Paldus 1988,1994).

Chapter 10

The Space Groups

The existence of crystalline structures in solids, makes solid state physics inseparable from the theory of space groups. The Hamiltonian of a perfect solid is invariant under the operations of a space group. Therefore the labels of irreps of a space group can be used to characterize the energy levels of a particle or quasi-particle in a crystal, as well as the electronic energy band structure and the phonon dispersion curves in crystalline solids. Knowledge about the irreps and the bases of space groups not only helps us to understand some properties of the solutions of the Hamiltonian, but also provides considerable simplification in the actual calculation of the eigenstates of a Hamiltonian.

The conventional rep theory of space groups is much more involved than that of point groups. The work on the determination of the irreps of a space group was started by Seitz in 1936. Thanks to the efforts of many scientists, tables of the irreps of the 230 space groups are now available (for example in Kovalev 1961, Miller 1967 (reprinted in Cracknell 1979), Bradley 1972). Programs for computing the irreps of space groups have been prepared (such as discussed in Worlton 1973, Neto 1975, Flodmark 1984, Ping 1989, Chen & Ping 1999).

The conventional approach to the space group rep theory is far from satisfactory. Firstly, the theory itself is rather complicated and elusive for one who only has a general knowledge of finite group representations. Secondly, the practical methods for constructing irreps of the little group are mainly Herring's little group method and the projective rep method (Bradley 1972, Birman 1974), or a variation of the projective-rep method (Kovalev 1958). The former two methods require the construction of reps for groups with high orders. For instance, for the projective-rep method, the order can be as high as 192 and 384 for the single-valued and double-valued reps respectively. Kovalev's approach is rather tedious. Thirdly, for many purposes, for example, for investigating symmetry change or symmetry-breaking in continuous phase transitions (Deonarine 1983), we need to use the irreducible basis adapted to a given group chain. Unfortunately, this requirement is not usually met by the existing tables or programs for the irreps of space groups.

In this chapter, we shall apply the theory of rep groups, introduced in Chapter 8, to space groups. We show that the problem of constructing the subgroup symmetry-adapted irreps for space groups is as easy as the equivalent problem for point groups.

10.1. The Euclidean Group

10.1.1. Definition of the Euclidean group

Suppose V_3 is a real Euclidean space in three dimensions. Let us find the transformations E

which keep the distance between any two points in V_3 unchanged, that is,

$$|E\mathbf{x} - E\mathbf{y}| = |\mathbf{x} - \mathbf{y}| \ . \tag{10-1}$$

E is called a length preserving transformation. All these transformations form a group $\mathbf{E}(3)$ known as the Euclidean group in three–dimensions.

The simplest elements in $\mathbf{E}(3)$ are translations $T_{\mathbf{a}}$:

$$T_{\mathbf{a}}\mathbf{x} = \mathbf{x} + \mathbf{a} \ . \tag{10-2}$$

Under the operation of $T_{\mathbf{a}}$, each point $\mathbf{x}$ in V_3 is shifted to $\mathbf{x} + \mathbf{a}$. All the translations $T_{\mathbf{a}}$ form a subgroup $\mathbf{T}(3)$ of the group $\mathbf{E}(3)$ known as the translation group. The translation group is Abelian, since

$$T_a T_b = T_b T_a = T_{a+b} \ . \tag{10-3}$$

Obviously, $T_{\mathbf{a}}^{-1} = T_{-\mathbf{a}}$.

We can easily find the translation operator $T_{\mathbf{a}}$ acting on a function $\psi(\mathbf{x})$. Consider an infinitesimal translation δx in the x direction. Under the operator $T_{\delta x}, \psi(x)$ becomes

$$\begin{aligned} \psi'(x) &= T_{\delta x}\psi(x) = \psi(T_{\delta x}^{-1}x) = \psi(x - \delta x) \\ &\cong \psi(x) - \frac{\partial \psi}{\partial x}\delta x \cong \exp(-\delta x \frac{\partial}{\partial x})\psi \ . \end{aligned} \tag{10-4}$$

From (10-4) the operator for a finite translation $\mathbf{a}$ can be deduced:

$$T_{\mathbf{a}} = \exp(-\mathbf{a} \cdot \nabla) = \exp(-i\hat{\mathbf{k}} \cdot \mathbf{a}) \ , \tag{10-5}$$

where $\hat{\mathbf{k}} = -\frac{1}{i}\nabla$ is the momentum operator (setting the Planck constant $\hbar = 1$) [compare this with the rotation operator $R_{\mathbf{n}}(\varphi) = \exp(-i\varphi \mathbf{J} \cdot \mathbf{n})$].

10.1.2. Properties of the Euclidean group operators

Suppose that E is an arbitrary element of $\mathbf{E}(3)$ and that $E\phi = \mathbf{a}$, where $\phi = (0,0,0)$ is the origin. Thus $T_{-\mathbf{a}}E\phi = \phi$, that is, $T_{-\mathbf{a}}E$ is the operation in $\mathbf{E}(3)$ which leaves the origin unchanged. We denote it by $\alpha = T_{-\mathbf{a}}E$. All the length preserving transformations which keep the origin unchanged form a group $\mathbf{O}(3)$, the orthogonal group in three dimensions. Since $\alpha = T_{-\mathbf{a}}E$, the group element E is uniquely expressed as

$$E = T_{\mathbf{a}}\alpha \ . \tag{10-6a}$$

We use the *Seitz notation* $\{\alpha|\mathbf{a}\}$ to represent a general element E of the group $\mathbf{E}(3)$, $\{\varepsilon|0\}$ represents the identity, and $\{\varepsilon|\mathbf{a}\}$ the translation $T_{\mathbf{a}}$. With this notation, (10-6a) becomes

$$\{\alpha|\mathbf{a}\} = \{\varepsilon|\mathbf{a}\}\{\alpha|0\} \ , \quad \{\varepsilon|\mathbf{a}\} \in \mathbf{T}(3), \{\alpha|0\} \in O(3) \ . \tag{10-6b}$$

The operation of $\{\alpha|\mathbf{a}\}$ on any vector $\mathbf{x}$ is defined by

$$\{\alpha|\mathbf{a}\}\mathbf{x} = \alpha\mathbf{x} + \mathbf{a} \ , \tag{10-7}$$

that is, perform the rotation α on the vector $\mathbf{x}$, followed by the translation $\mathbf{a}$. Using

$$\{\alpha|\mathbf{a}\}\{\beta|\mathbf{b}\}\mathbf{x} = \{\alpha|\mathbf{a}\}(\beta\mathbf{x} + \mathbf{b}) = \alpha\beta\mathbf{x} + \alpha\mathbf{b} + \mathbf{a} \ , \tag{10-8}$$

we obtain the multiplication law

$$\{\alpha|\mathbf{a}\}\{\beta|\mathbf{b}\} = \{\alpha\beta|\alpha\mathbf{b} + \mathbf{a}\} \ . \tag{10-9}$$

Setting $\{\alpha\beta|\alpha\mathbf{b}+\mathbf{a}\}=\{\varepsilon|0\}$, we find the inverse element of $\{\alpha|\mathbf{a}\}$,

$$\{\alpha|\mathbf{a}\}^{-1}=\{\alpha^{-1}|-\alpha^{-1}\mathbf{a}\}\ . \tag{10-10}$$

From (10-9) we have

$$\{\alpha|\mathbf{a}\}=\{\varepsilon|\mathbf{a}\}\{\alpha|0\}=\{\alpha|0\}\{\varepsilon|\alpha^{-1}\mathbf{a}\}\ . \tag{10-11}$$

Thus translations and rotations (or rotation–reflections) do not commute, unless the translation vector $\mathbf{a}$ is parallel to the rotation axis or the reflection plane, that is,

$$[\{\varepsilon|\mathbf{a}\},\{\alpha|0\}]=0,\ \text{when}\ \mathbf{a}\,\|\,\text{the rotation axis of}\ \alpha\ , \tag{10-12a}$$

$$[\{\varepsilon|\mathbf{a}\},\{\sigma|0\}]=0,\ \text{when}\ \mathbf{a}\,\|\,\text{the reflection plane}\ \sigma\ . \tag{10-12b}$$

From (10-9) we also have

$$\{\alpha|\mathbf{a}+\mathbf{b}\}=\{\varepsilon|\mathbf{a}\}\{\alpha|\mathbf{b}\}=\{\alpha|\mathbf{b}\}\{\varepsilon|\alpha^{-1}\mathbf{a}\}\ . \tag{10-13}$$

With the Seitz notation, (10-5) is rewritten as

$$\{\varepsilon|\mathbf{a}\}=\exp(-\mathbf{a}\cdot\nabla)=\exp(-i\hat{\mathbf{k}}\cdot\mathbf{a})\ . \tag{10-14}$$

10.2. The Lattice Group

A crystal is formed by arranging atoms or ions in a space lattice

$$L=\{\mathbf{R}_n\}\ , \tag{10-15a}$$

called an *empty lattice*, defined by the set of points (the lattice points)

$$\mathbf{R}_n=n_1\mathbf{t}_1+n_2\mathbf{t}_2+n_3\mathbf{t}_3\ , \tag{10-15b}$$

with integers n_i. The vectors $\mathbf{t}_i$ are called *primitive translations* and must not be coplanar. $\mathbf{R}_n$ is called a *lattice vector*. The parallelepiped defined by $\mathbf{t}_1,\mathbf{t}_2$ and $\mathbf{t}_3$ is called the *primitive cell*. Notice that atoms or ions are not necessarily at the lattice points, and generally an array of atoms or ions with a specific relative orientation is associated with each lattice point.

The basis vectors $\mathbf{t}_1,\mathbf{t}_2$ and $\mathbf{t}_3$ are in general not orthogonal to each other. Their scalar product, or equivalently the metric tensor, is designated by

$$g_{ij}=\mathbf{t}_i\cdot\mathbf{t}_j\ . \tag{10-16}$$

All the rotations α which keep $\mathbf{R}_n$ in the lattice $\{\mathbf{R}_n\}$ form a point group $\mathbf{P}$ which is referred to as the *point group of the empty lattice*, or the *holosymmetric point group* of the crystal system,

$$\mathbf{P}=\{\alpha:\alpha\mathbf{R}_n\in L\}\ . \tag{10-17}$$

The point group $\mathbf{P}$ always contains the space inversion operator I, since if $\mathbf{R}_n$ is a lattice vector, so is $-\mathbf{R}_n$.

The translation group with the lattice vectors $\mathbf{R}_n$ as translation vectors is called the *lattice group* and is denoted by

$$\mathbf{T}=\{\{\varepsilon|\mathbf{R}_n\}\}\ . \tag{10-18}$$

Obviously, the lattice group is a subgroup of the symmetry group of an infinite crystal, since any point $\mathbf{x}$ in the crystal is equivalent to the points $\mathbf{x}+\mathbf{R}_n$. In reality a crystal is finite but contains a very large number of atoms, $\sim 10^{20}$ per cm^3. Therefore it can be treated as an

infinite crystal if what we are concerned with are the bulk properties of the material, such as conductivity and specific heat.

10.3. The Space Group

Together with translation symmetry, a crystal also possesses certain kinds of rotation and reflection symmetries. The complete symmetry group of a crystal is called the *space group*, designated **G**. The space group is a subgroup of the Euclidean group, whereas the lattice group is a subgroup of the space group, that is $\mathbf{E}(3) \supset \mathbf{G} \supset \mathbf{T}$. An element of a space group **G** is designated by

$$\{\alpha|\mathbf{a}\} = \{\alpha|\mathbf{V}(\alpha) + \mathbf{R}_n\} , \tag{10-19a}$$

where the vector $\mathbf{V}(\alpha)$ associated with the rotation α is called a *non-primitive*, or *fractional translation*. $\mathbf{V}(\alpha)$ is either zero or a translation which is less than a lattice vector. We always associate $\mathbf{V}(\varepsilon) = 0$ with the identity rotation ε. α is a rotation operator (proper or improper) belonging to the so-called *isogonal point group* $\mathbf{G}_0$ of the space group. As we have said, a crystal is formed by arranging a collection of atoms or ions in an empty lattice. Since both the arrangement and the ions have some symmetries of their own, the crystal point group $\mathbf{G}_0$ has a lower symmetry than the point group **P** of the empty lattice, unless the arrangement as well as the ions have a symmetry no lower than that of **P**. In other words, in general $\mathbf{G}_0$ is a subgroup of **P**.

A space group **G** is designated by

$$\mathbf{G} = \{\{|\alpha|\mathbf{a}\}\} = \{\{\alpha|\mathbf{V}(\alpha) + \mathbf{R}_n\} : \alpha \in \mathbf{G}_0, \mathbf{R}_n \in L\} . \tag{10-19b}$$

Space groups can be divided into two types. The first ones are those for which $\mathbf{V}(\alpha) = 0$ for every α. These are called *simple* or *symmorphic space groups*. There are 73 symmorphic space groups. Clearly, the point group $\mathbf{G}_0 = \{\alpha\}$ is a subgroup of the symmorphic space group.

The others are those for which not all $\mathbf{V}(\alpha)$ are zeroes, called *non-symmorphic space groups*. There are 157 non-symmorphic space groups. Notice that the crystal point group $\mathbf{G}_0$ is not a subgroup of the non-symmorphic space group. A space group element $\{\alpha|\mathbf{V}(\alpha)\}$ with nonzero $\mathbf{V}(\alpha)$ is called a *screw rotation* if α is a rotation, or a *glide reflection* if α is a reflection.

Let us study the restrictions on the non-primitive translations.

Suppose α is an n-fold axis C_n with a non-primitive translation **V** in parallel with the axis. $\{C_n|0\}$ and $\{\varepsilon|\mathbf{V}\}$ commute on account of (10-12). Therefore

$$\{C_n|\mathbf{V}\}^n = \{C_n^n|n\mathbf{V}\} = \{\varepsilon|n\mathbf{V}\} . \tag{10-20}$$

Thus $n\mathbf{V} = l\mathbf{R}_m$, where $\mathbf{R}_m$ is the shortest lattice vector along the direction of the C_n axis, and **V** takes the following form

$$\mathbf{V} = \frac{l}{n}\mathbf{R}_m , \quad l = 0, 1, 2, \ldots, n-1 . \tag{10-21}$$

Similarly, if σ is a reflection plane with a non-primitive translation **V** parallel with the plane, then

$$\mathbf{V} = \frac{1}{2}\mathbf{R}_m , \tag{10-22}$$

$\mathbf{R}_m$ being the shortest lattice vector in the direction of **V**.

The non-primitive translations of the 157 non-symmorphic space groups are of the following general form

$$\mathbf{V} = \tfrac{1}{m}(m_1\mathbf{t}_1 + m_2\mathbf{t}_2 + m_3\mathbf{t}_3) , \tag{10-23}$$

$m = 2,3,4,5,6; m_i = 0,1,\ldots,m-1$. The space group is a discrete infinite group. However, to define a space group, it suffices to give the primitive translation $\mathbf{t}_i$ and a finite number of elements $\{\alpha|\mathbf{V}(\alpha)\}$.

From the multiplication rule

$$\{\alpha|\mathbf{V}(\alpha)+\mathbf{R}_n\}\{\beta|\mathbf{V}(\beta)+\mathbf{R}_m\} = \{\alpha\beta|\alpha\mathbf{V}(\beta)+\mathbf{V}(\alpha)+\alpha\mathbf{R}_m+\mathbf{R}_n\}\ , \tag{10-24}$$

one infers that the lattice vectors and non–primitive translations must satisfy the following conditions,

$$\alpha\mathbf{R}_m = \mathbf{R}_l, \quad \mathbf{R}_l \in L\ , \tag{10-25a}$$

$$\mathbf{V}(\alpha)+\alpha\mathbf{V}(\beta) = \mathbf{V}(\alpha\beta)+\mathbf{R}_{\alpha\beta}\ . \tag{10-25b}$$

From

$$\{\alpha|\mathbf{a}\}\{\varepsilon|\mathbf{R}_n\}\{\alpha^{-1}|-\alpha^{-1}\mathbf{a}\} = \{\varepsilon|\alpha\mathbf{R}_n\}\ , \tag{10-26}$$

and (10-25a), we see that the lattice group $\mathbf{T}$ is an invariant subgroup of the space group.

A symmorphic space group $\mathbf{G}$ is a semi–direct product of the lattice group and the crystal point group, $\mathbf{G} = \mathbf{T} \wedge \mathbf{G}_0$.

10.4. The Point Group P and the Crystal System

It can be seen from Eq. (10-25a) that the primitive translations $\mathbf{t}_1, \mathbf{t}_2$ and $\mathbf{t}_3$ span a three–dimensional rep of the point group $\mathbf{G}_0$,

$$\alpha\mathbf{t}_i = \sum_{j=1}^{3} D_{ji}(\alpha)\mathbf{t}_j\ . \tag{10-27}$$

On account of $\alpha\mathbf{t}_i$ belonging to the lattice L, we have $\alpha\mathbf{t}_i = n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3$. Therefore the matrix elements[1] $D_{ji}(\alpha)$ in (10-27), as well as the characters $\chi(\alpha)$ are integers. The effect of the point–group operations α on the primitive translations $\mathbf{t}_i$ is given in Table 10.21-2 (taken from Bradley 1972, Table 3.2, pp. 84). On the other hand, (801) and (8-20) tell us that in the Cartesian basis $\mathbf{i},\mathbf{j},\mathbf{k}$ the character of rotation operator is $\chi(\varphi) = \pm 1 + 2\cos\varphi, \varphi$ being the rotation angle, and $+1$ (-1) correspond to proper (improper) rotations. Since the bases $(\mathbf{t}_1,\mathbf{t}_2,\mathbf{t}_3)$ and $(\mathbf{i},\mathbf{j},\mathbf{k})$ differ only by a similarity transformation, and the character is invariant under a similarity transformation, we immediately arrive at the condition for the allowable rotation angles,

$$\pm 1 + 2\cos\varphi = \text{integer}\ . \tag{10-28}$$

Thus φ can only take on the values $2\pi/n, n = 1,2,3,4,6$. In other words, the group $\mathbf{P}$ can only contain 1–, 2–, 3–, 4– and 6–fold axes. Among the point groups, only the 32 crystal point groups fulfill this requirement. They include the cyclic groups $\mathcal{C}_n, n = 1,2,3,4,6$; the D_n groups, $n = 2,3,4,6$; the tetrahedral group T and the octahedral group O. The inclusion of inversion and reflection results in the groups $\mathcal{C}_i, S_4, S_6; \mathcal{C}_{nh}, n = 1,2,3,4,6; \mathcal{C}_{nv}$ and $D_{nh}, n = 2,3,4,6; D_{2d}, D_{3d}, T_d, T_h$ and O_h.

Apart from the restriction (10-28), the following theorem imposes another constraint on the permissible point groups $\mathbf{P}$ of the empty lattice.

Theorem 10.1: If the point group $\mathbf{P}$ of an empty lattice contains an n–fold axis $C_n, n > 2$, then it necessarily contains the group $\mathcal{C}_{nv}$. (See Tao 1986 for a proof).

As a result of this restriction, only seven among the 32 crystal point groups survive. They are $\mathcal{C}_i, \mathcal{C}_{2h} = \mathcal{C}_2 \times \mathcal{C}_i, D_{2h} = D_2 \times \mathcal{C}_i, D_{3d} = D_3 \times \mathcal{C}_i, D_{4h} = D_4 \times \mathcal{C}_i, D_{6h} = D_6 \times \mathcal{C}_i$ and $O_h = O \times \mathcal{C}_i$.

[1] Since $\mathbf{t}_i$ are not orthogonal, the rep matrix $D(\alpha)$ of the unitary operator α is not a unitary matrix.

These are the only allowable point groups $\mathbf{P}$ of the empty lattice, and as expected, they all contain the inversion I. Their interrelation is as follows

$$\begin{array}{ccccccc} O_h & \supset & D_{4h} & \supset & D_{2h} & \supset & C_{2h} & \supset & C_i \\ & & & & \cap & & \cap & & \\ & & & & D_{6h} & & D_{3d} & & \end{array} \quad . \tag{10-29}$$

Definition 10.1: Two empty lattices are said to belong to the same crystal system if they have the same symmetry point group $\mathbf{P}$.

Thus there are only seven crystal systems. Their names and the conventional forms of the related metric tensors are

$$\begin{array}{llll} \text{Triclinic} & \text{Monoclinic} & \text{Orthorhomic} & \text{Tetragonal} \\ \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix}, & \begin{pmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{pmatrix}, & \begin{pmatrix} g_{11} & 0 & 0 \\ 0 & g_{22} & 0 \\ 0 & 0 & g_{33} \end{pmatrix}, & \begin{pmatrix} a & b & b \\ b & a & b \\ b & b & a \end{pmatrix}, \end{array} \tag{10-30}$$

$$\begin{array}{lll} \text{Trigonal} & \text{Hexagonal} & \text{Cubic} \\ \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & c \end{pmatrix}, & \begin{pmatrix} a & -a/2 & 0 \\ -a/2 & 0 & 0 \\ 0 & 0 & c \end{pmatrix}, & \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix}. \end{array}$$

10.5. The Bravais Lattices

In the previous section, we discussed the restriction on the allowable point groups $\mathbf{P}$ imposed by the symmetry of the empty lattice. Conversely, the point group $\mathbf{P}$ will also impose restrictions on the possible types of the empty lattices.

Definition 10.2: Two lattices belonging to the same crystal system are said to be of the same type if one of them can be obtained from the other by a continuous deformation such that the Bravais lattice does not undergo a transformation passing through a crystal system of lower symmetry.

For example, the face-oriented cubic Bravais lattice Γ_c^f cannot be deformed into a body-centered cubic Bravais lattice Γ_c^v without passing through the trigonal Bravais lattice. Therefore Γ_c^f and Γ_c^v are of different types.

The seven crystal systems contain 14 types of lattices, called the 14 *Bravais lattices.* Their names, geometric forms along with the primitive translations are given in Fig. 10.5. With these primitive translations one can calculate the metric tensor g_{ij} associated with a given Bravais lattice. For instance, for the cubic system we have

$$a^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \frac{a^2}{4} \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}, \quad \frac{a^2}{4} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}. \tag{10-31}$$

It can be shown that from the 14 Bravais lattices $\{\mathbf{R}_n\}$, the 32 crystal point groups $\mathbf{G}_0 = \{\alpha\}$, and the various kinds of possible non-primitive translations $\mathbf{V}(\alpha)$, one can construct a total of 230 space groups $\mathbf{G} = \{\alpha|\mathbf{V}(\alpha) + \mathbf{R}_n\}$. These space groups are divided into 32 classes on the basis of the crystal point groups $\mathbf{G}_0$. We use the Schönflies symbol (standing for point group) with superscript to denote a space group. For example, there are 10 space groups associated with the point group O_h and they are designated as $O_h^1, \ldots, O_h^{10}$.

The generators of the 230 space groups are given by Bradley (1972, Table 3.7, pp. 127).

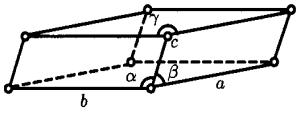
The distribution of the 32 crystal groups among the seven crystal systems is as follows.

1. Triclinic: $\mathbf{P} = \mathcal{C}_i$; $\mathbf{G}_0 = \mathcal{C}_i, \mathcal{C}_1$
2. Monoclinic: $\mathbf{P} = \mathcal{C}_{2h}$; $\mathbf{G}_0 = \mathcal{C}_{2h}, \mathcal{C}_2, \mathcal{C}_s$
3. Orthorhombic: $\mathbf{P} = D_{2h}$; $\mathbf{G}_0 = D_{2h}, D_2, \mathcal{C}_{2v}$
4. Trigonal: $\mathbf{P} = D_{3d}$; $\mathbf{G}_0 = D_{3d}, D_3, \mathcal{C}_{3v}, \mathcal{C}_3, S_6$
5. Tetragonal: $\mathbf{P} = D_{4h}$; $\mathbf{G}_0 = D_{4h}, D_{4d}, D_4, \mathcal{C}_{4v}, S_4, \mathcal{C}_4, D_{2d}$
6. Hexagonal: $\mathbf{P} = D_{6h}$; $\mathbf{G}_0 = D_{6h}, D_6, \mathcal{C}_{6h}, \mathcal{C}_{6v}, \mathcal{C}_6, D_{3h}, \mathcal{C}_{3h}$
7. Cubic: $\mathbf{P} = O_h$; $\mathbf{G}_0 = O_h, O, T_d, T, T_h$.

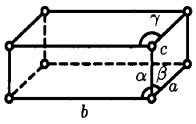
Fig. 10.5. The 14 Bravais lattices.

In the following a, b and c represent the lengths of the three sides, while α,β and γ represent the angles between the sides **b** and **c**, **c** and **a**, and **a** and **b**, respectively.

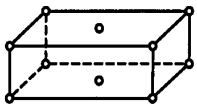
1. Triclinic — $P(\Gamma_t), \mathbf{P} = \mathcal{C}_i$.
   $a \neq b \neq c$
   $\alpha \neq \beta \neq \gamma$



2. Monoclinic $a \neq b \neq c, \alpha = \beta = \pi/2 \neq \gamma, \mathbf{P} = \mathcal{C}_{2h}$

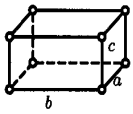


Simple Γ_m
Monoclinic — P
$\mathbf{t}_i$:(0,−b,0);(a sin γ,−a cos γ,0);
(0,0,c).

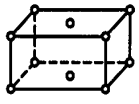


Base-centered Γ_m^b
Monoclinic — B
$\mathbf{t}_i$:(0,−b,0);$\frac{1}{2}$(a sin γ,−a cos γ,−c);
$\frac{1}{2}$(a sin γ,−a cos γ,c).

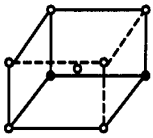
3. Orthorhombic $a \neq b \neq c, \alpha = \beta = \gamma = \pi/2, \mathbf{P} = D_{2h}$



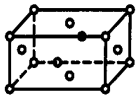
Simple Γ_0
Orthorhombic — P
$\mathbf{t}_i$:(0,−b,0);
(a,0,0);
(0,0,c).



Base-centered Γ_0^b
Orthorhombic — C
$\mathbf{t}_i$:$\frac{1}{2}$(a,−b,0);
$\frac{1}{2}$(a,b,0);
(0,0,c).



Body-centered Γ_0^v
Orthorhombic — I
$\mathbf{t}_i$:$\frac{1}{2}$(a,b,c);
$\frac{1}{2}$(−a,−b,c);
$\frac{1}{2}$(a,−b,−c).



Face-centered Γ_0^f
Orthorhombic — F
$\mathbf{t}_i$:$\frac{1}{2}$(a,0,c);
$\frac{1}{2}$(0,−b,c);
$\frac{1}{2}$(a,−b,0).

4. Trigonal — $R(\Gamma_{rh}), \mathbf{P} = D_{3d}$.
   $a = b \neq c$,
   $\alpha = \beta = \gamma < 2\pi/3$,
   $\alpha \neq \pi/2$.
   $\mathbf{t}_i : (0, -a, c); \frac{1}{2}(\sqrt{3}\,a, a, 2c); \frac{1}{2}(-\sqrt{3}\,a, a, 2c)$.

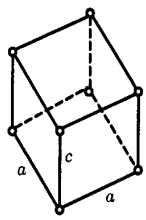
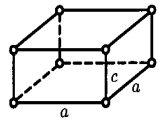
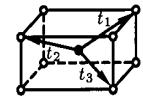


Fig. 10.5. continued

5. Tetragonal, $a = b \neq c, \alpha = \beta = \gamma = \pi/2, \mathbf{P} = D_{4h}$.

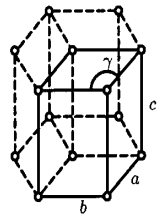


Simple Γ_q
Tetragonal — P
$\mathbf{t_i}$:(a,0,0);(0,a,0);(0,0,c).

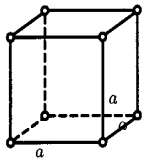


Base-centered Γ_q^v
Tetragonal — I
$\mathbf{t_i}$:$\frac{1}{2}(-a,a,c)$;$\frac{1}{2}(a,-a,c)$;$\frac{1}{2}(a,a,-c)$.

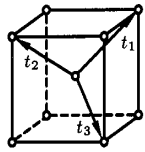
6. Hexagonal — P, $\Gamma_h, \mathbf{P} = D_{6h}$
$a = b \neq c, \alpha = \beta = \pi/2, \gamma = 2\pi/3$.
$\mathbf{t}_i : (0, -a, 0);\ \frac{1}{2}(\sqrt{3}\,a, a, 0);\ \frac{1}{2}(0, 0, c)$.



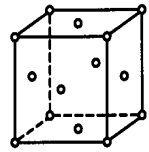
7. Cubic, $\mathbf{P} = O_h, a = b = c, \alpha = \beta = \gamma = \pi/2$.



Simple Γ_c
Cubic — P
$\mathbf{t_i}$:(a,0,0);(0,a,0);
(0,0,a).



Body-centered Γ_c^v
Cubic — I
$\mathbf{t_i}$:$\frac{1}{2}(-a,a,a)$;$\frac{1}{2}(a,-a,a)$;
$\frac{1}{2}(a,a,-a)$.



Face-centered Γ_c^f
Cubic — F
$\mathbf{t_i}$:$\frac{1}{2}(0,a,a)$;$\frac{1}{2}(a,0,a)$;
$\frac{1}{2}(a,a,0)$.

10.6. Operators of the Space Group

10.6.1. The properties of group operators

It must be emphasized that the operators of the Euclidean group or the space group are not linear if they are regarded as coordinate transformation operators. To show this it suffices to consider the translation operators $T_{\mathbf{a}}$. Suppose $\mathbf{z} = c_1\mathbf{x} + c_2\mathbf{y}$, where c_1 and c_2 are arbitrary constants. From (10-2),

$$T_{\mathbf{a}}\mathbf{z} = c_1\mathbf{x} + c_2\mathbf{y} + \mathbf{a}\ . \tag{10-32a}$$

If the operator $T_{\mathbf{a}}$ were a linear operator, it should have been

$$T_{\mathbf{a}}\mathbf{z} = c_1 T_{\mathbf{a}}\mathbf{x} + c_2 T_{\mathbf{a}}\mathbf{y} = c_1\mathbf{x} + c_2\mathbf{y} + (c_1 + c_2)\mathbf{a}\ . \tag{10-32b}$$

However $(c_1 + c_2)\mathbf{a} \neq \mathbf{a}$. Therefore, the coordinate transformation operators $T_{\mathbf{a}}$ are not linear.

Nevertheless, the operators of a space group are linear if they are defined as the *substitutional operators* in a function space, that is,

$$\{\alpha|\mathbf{a}\}\psi(x) = \psi(\{\alpha|\mathbf{a}\}^{-1}\mathbf{x}) = \psi(\alpha^{-1}(\mathbf{x} - \mathbf{a}))\ . \tag{10-33}$$

To show this, it again suffices to consider the translational operators. Suppose

$$T_{\mathbf{a}}\psi(\mathbf{x}) = \psi(\mathbf{x} - \mathbf{a})\ ,$$

then we have

$$T_{\mathbf{a}}[c_1\psi(\mathbf{x}) + c_2\varphi(\mathbf{x})] = c_1\psi(\mathbf{x}-\mathbf{a}) + c_2\varphi(\mathbf{x}-\mathbf{a}) = c_1T_{\mathbf{a}}\psi(\mathbf{x}) + c_2T_{\mathbf{a}}\varphi(\mathbf{x}) \ .$$

Therefore the operator $T_{\mathbf{a}} = \{\varepsilon|\mathbf{a}\}$ is linear under the definition of (10-33). The same is true for the operator $\{\alpha|\mathbf{a}\}$.

With this definition, the multiplication rule for the group elements is identical to (10-9) which was used in coordinate space; that is

$$\begin{aligned}\{\alpha|\mathbf{a}\}\{\beta|\mathbf{b}\}\psi(\mathbf{x}) &= \{\alpha|\mathbf{a}\}\psi(\beta^{-1}\mathbf{x}-\beta^{-1}\mathbf{b}) = \psi(\beta^{-1}\{\alpha|\mathbf{a}\}^{-1}\mathbf{x}-\beta^{-1}\mathbf{b}) \\ &= \psi(\{\alpha\beta|\alpha\mathbf{b}+\mathbf{a}\}^{-1}\mathbf{x}) = \{\alpha\beta|\alpha\mathbf{b}+\mathbf{a}\}\psi(\mathbf{x}) \ . \qquad (10\text{-}34a)\end{aligned}$$

It is worth mentioning that in performing the operations in (10-34a) and the like, one must be very careful to notice the following points:

$$\{\varepsilon|\mathbf{a}\}\psi(\alpha^{-1}\mathbf{x}) = \psi(\alpha^{-1}(\mathbf{x}-\mathbf{a})) \neq \psi(\alpha^{-1}\mathbf{x}-\mathbf{a}) \ , \qquad (10\text{-}34b)$$

$$\{\alpha|0\}\psi(\mathbf{x}-\mathbf{b}) = \psi(\alpha^{-1}\mathbf{x}-\mathbf{b}) \neq \psi(\alpha^{-1}(\mathbf{x}-\mathbf{b})) \ , \qquad (10\text{-}34c)$$

$$\{\alpha|0\}\psi(\beta^{-1}\mathbf{x}) = \psi(\beta^{-1}\alpha^{-1}\mathbf{x}) \neq \psi(\alpha^{-1}\beta^{-1}\mathbf{x}) \ . \qquad (10\text{-}34d)$$

Equation (10-33) can be rewritten as

$$\{\alpha|\mathbf{a}\}\psi(\mathbf{x}) = \psi(\mathbf{x}'-\mathbf{a}') \ , \quad \mathbf{x}'-\mathbf{a}' = \alpha^{-1}(\mathbf{x}-\mathbf{a}) \ , \qquad (10\text{-}35a)$$

or in component form

$$x_i' - a_i' = \sum_{j=1}^{3} D_{ij}(\alpha^{-1})(x_j - a_j) = \sum_{j=1}^{3} D_{ji}(\alpha)(x_j - a_j) \ , \qquad (10\text{-}35b)$$

where $D_{ij}(\alpha)$ are the matrix elements of the point-group operator α in the rep carried by the basis functions x, y and z.

Henceforth we will use only the definition (10-35).

10.6.2. Example: The group D_{4h}^{14}

As an example we will give the operators of the space group D_{4h}^{14}. It is the symmetry group of the crystal TiO_2. TiO_2 belongs to the tetragonal system and the arrangement of its atoms is shown in Fig. 10.6-1. Although there is a TiO_2 molecule in the center of each primitive cell, it belongs to the simple tetragonal instead of the body–centered tetragonal, since the molecule in the center has a different orientation from that of the molecules in the corners.

The group operators of D_{4h}^{14} are as follows:

1. The pure translations

$$\mathbf{R}_n = n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3 \ ,$$

where $\mathbf{t}_1, \mathbf{t}_2$ and $\mathbf{t}_3$ are mutually orthogonal and $t_1 = t_2 = a, t_3 = c$.

2. The operations belonging to the point group D_{2h} (see Fig. 10.6-2)

$$\begin{aligned}D_{2h}: &\{\varepsilon|0\}, \{C_{2z}|0\}, \{C_{2a}|0\}, \{C_{2b}|0\} \ , \\ &\{I|0\}, \{\sigma_z|0\}, \{\sigma_a|0\}, \{\sigma_b|0\} \ .\end{aligned}$$

3. The operators involving non–primitive translations

$$\begin{aligned}&\{C_{4x}^{+}|\mathbf{v}\} \ , \quad \{C_{4z}^{-}|\mathbf{v}\} \ , \quad \{C_{2x}|\mathbf{v}\} \ , \quad \{C_{2y}|\mathbf{v}\} \ , \\ &\{S_{4z}^{-}|\mathbf{v}\} \ , \quad \{S_{4z}^{+}|\mathbf{v}\} \ , \quad \{\sigma_x|\mathbf{v}\} \ , \quad \{\sigma_y|\mathbf{v}\} \ , \quad \mathbf{v} = \frac{1}{2}(\mathbf{t}_1 + \mathbf{t}_2 + \mathbf{t}_3) \ .\end{aligned}$$

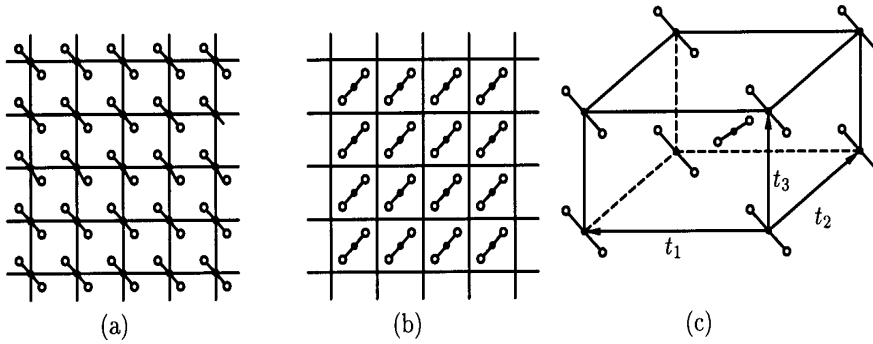


Fig. 10.6-1. The arrangement of atoms in TiO_2 and the primitive cell of D_{4h}^{14}.
We use • to denote a Ti atom and ○ to denote an O atom. The three subfigures are;
(a) The atoms in the layers 1,3,...
(b) The atoms in the layers 0,2,4,...
(c) The primitive cell of D_{4h}^{14}.

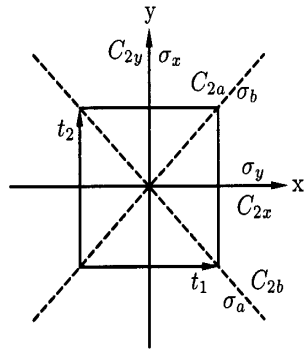


Fig.10.6-2. The group D_{2h}.

According to (10-35) and the matrix elements of point-group operators (such as (8-1) and (8-20)), we obtain Table 10.6 for the action of the group elements of D_{4h}^{14} on a function $\psi(x,y,z)$.

10.7. The Reciprocal Lattice Vectors

Let $(\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3)$ be a set of non-orthonormal basis vectors. According to (2-15a), we can introduce another set of dual basis vectors $(\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$, so that

$$\mathbf{b}_i \cdot \mathbf{t}_j = 2\pi\delta_{ij} \ , \tag{10-36}$$

where the factor 2π is introduced for convenience. It is easily seen that the relation between $\mathbf{b}_i$ and $\mathbf{t}_i$ is

$$\mathbf{b}_i = 2\pi(\mathbf{t}_j \times \mathbf{t}_k)/[\mathbf{t}_i \cdot (\mathbf{t}_j \times \mathbf{t}_k)], \quad i,j,k \quad \text{cyclic.} \tag{10-37}$$

From (5-12c) we know that $\mathbf{t}_i$ is the covariant basis, while $\mathbf{b}_i$ is the contravariant basis, and $\mathbf{b}_i \cdot \mathbf{t}_j = 2\pi\delta_{ij}$ is an invariant. The metric tensor for the contravariant basis is

$$g^{ij} = \mathbf{b}_i \cdot \mathbf{b}_j \ . \tag{10-38}$$

According to (5-12b), we have

$$|g^{ij}| = 4\pi^2 |g_{ij}|^{-1} \ . \tag{10-39}$$

Table 10.6. The action of the group elements of the space group D_{4h}^{14} on a function $\psi(x,y,z)$.*

$\{\alpha\|\mathbf{a}\}$ $\{\alpha\|\mathbf{a}\}\psi$	$\{\epsilon\|0\}$ $\psi(x,y,z)$	$\{C_{2a}\|0\}$ $\psi(y,x,-z)$	$\{C_{2b}\|0\}$ $\psi(-y,-x,-z)$	$\{C_{2z}\|0\}$ $\psi(-x,-y,z)$	$\{C_{4z}^{+}\|\mathbf{v}\}$ $\psi(\eta,-\xi,\zeta)$	$\{C_{4z}^{-}\|\mathbf{v}\}$ $\psi(-\eta,\xi,\zeta)$
$\{\alpha\|\mathbf{a}\}$ $\{\alpha\|\mathbf{a}\}\psi$	$\{\mathbf{I}\|0\}$ $\psi(-x,-y,-z)$	$\{\sigma_a\|0\}$ $\psi(-y,-x,z)$	$\{\sigma_b\|0\}$ $\psi(y,x,z)$	$\{\sigma_z\|0\}$ $\psi(x,y,-z)$	$\{S_{4z}^{-}\|\mathbf{v}\}$ $\psi(-\eta,\xi,-\zeta)$	$\{S_{4z}^{+}\|\mathbf{v}\}$ $\psi(\eta,-\xi,-\zeta)$
$\{\alpha\|\mathbf{a}\}$ $\{\alpha\|\mathbf{a}\}\psi$	$\{C_{2x}\|\mathbf{v}\}$ $\psi(\xi,-\eta,-\zeta)$	$\{C_{2y}\|\mathbf{v}\}$ $\psi(-\xi,\eta,-\zeta)$	$\{\sigma_x\|\mathbf{v}\}$ $\psi(-\xi,\eta,\zeta)$	$\{\sigma_y\|\mathbf{v}\}$ $\psi(\xi,-\eta,\zeta)$	$\{\epsilon\|\mathbf{R}_n\}$ $\psi(x-n_1a,y-n_2a,z-n_3c)$	

*$\xi = x - \frac{1}{2}, \eta = y - \frac{1}{2}, \zeta = z - \frac{1}{2}$.

Let us define

$$\mathbf{K}_m = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3 \ , \tag{10-40a}$$

with integers m_i. The $\mathbf{K}_m$ are referred to as the reciprocal lattice vectors, and the lattice formed by the vectors $\mathbf{K}_m$ is called the *reciprocal lattice*, denoted

$$L^{-1} = \{\mathbf{K}_m\} \ . \tag{10-40b}$$

We first prove that the reciprocal lattice and the space lattice have the same symmetry point group $\mathbf{P}$. From (10-15b), (10-40a) and (10-36), it follows that

$$\mathbf{K}_m \cdot \mathbf{R}_n = 2\pi \sum_{i=1}^{3} n_i m_i = 2\pi \times \text{integer} \ . \tag{10-41a}$$

Since $\alpha^{-1}\mathbf{R}_n$ is a lattice vector, $\mathbf{K}_m \cdot \alpha^{-1}\mathbf{R}_n = 2\pi\times$ integer. Using the unitarity of the operator α, one has

$$\mathbf{K}_m \cdot \alpha^{-1}\mathbf{R}_n = \alpha\mathbf{K}_m \cdot \mathbf{R}_n = 2\pi \times \text{integer} \ .$$

The above relation holds for any $\mathbf{R}_n$, thus $\alpha\mathbf{K}_m$ is also a reciprocal lattice vector,

$$\alpha\mathbf{K}_m = \mathbf{K}_l \ . \tag{10-41b}$$

Consequently, the space lattice and its reciprocal lattice must belong to the same crystal system. However they are not necessarily of the same type. Actually, they are of the same type except for the cubic and orthorhombic crystal systems, for which the reciprocal lattice of the body-centered space lattice is face-centered and vice versa. For the cubic, this can be seen from the following equation,

$$g_I = \frac{a^4}{4} g_F^{-1} \ , \tag{10-42}$$

where (10-31) has been used. Equation (10-42) agrees with the condition (10-39) apart from a trivial constant factor. Table 10.7 lists the cases for which the reciprocal lattices and their space lattices belong to different crystal types.

10.8. Irreps of the Lattice Group

With the $\mathbf{t}_i$ as our basis,

$$\mathbf{r} = \xi_1\mathbf{t}_1 + \xi_2\mathbf{t}_2 + \xi_3\mathbf{t}_3 \ . \tag{10-43}$$

In analogy with (10-4) we have

$$\begin{aligned} \{\varepsilon|\delta\xi_1\mathbf{t}_1\}\psi(\xi_1) = \psi(\xi_1 - \delta\xi_1) &\cong \exp\left[-\delta\xi_1 \frac{\partial}{\partial\xi_1}\right]\psi(\xi_1) \\ &= \exp\left[-(\delta\xi_1\mathbf{t}_1)\cdot\frac{1}{2\pi}\left(\frac{\partial}{\partial\xi_1}\mathbf{b}_1\right)\right]\psi(\xi_1) \ . \end{aligned} \tag{10-44}$$

Table 10.7. The correspondence between the reciprocal lattices and space lattices when they are of different types.

crystal system	space lattice	reciprocal lattice
orthorhombic	body-centered	face-centered
	face-centered	body-centered
cubic	body-centered	face-centered
	face-centered	body-centered

Thus we have the translation operator

$$\{\varepsilon|\mathbf{R}_n\} = \exp(-i\hat{\mathbf{k}}\cdot\mathbf{R}_n) = \exp\left[-\left(n_1\frac{\partial}{\partial\xi_1} + n_2\frac{\partial}{\partial\xi_2} + n_3\frac{\partial}{\partial\xi_3}\right)\right] , \tag{10-45a}$$

$$\hat{\mathbf{k}} = -i\nabla = -\frac{i}{2\pi}\left(\frac{\partial}{\partial\xi_1}\mathbf{b}_1 + \frac{\partial}{\partial\xi_2}\mathbf{b}_2 + \frac{\partial}{\partial\xi_3}\mathbf{b}_3\right) . \tag{10-45b}$$

The lattice group is Abelian, hence the group operator is just the class operator. Its CSCO can be chosen as the set of group operators $\{\varepsilon|\mathbf{R}_n\} = \exp(-i\hat{\mathbf{k}}\cdot\mathbf{R}_n)$. The irreducible bases of the lattice group are eigenfunctions of the CSCO,

$$\{\varepsilon|\mathbf{R}_n\}\psi_{\mathbf{k}} = \exp(-i\hat{\mathbf{k}}\cdot\mathbf{R}_n)\psi_{\mathbf{k}} = \exp(-i\mathbf{k}\cdot\mathbf{R}_n)\psi_{\mathbf{k}} , \tag{10-46}$$

where $\mathbf{k}$ are eigenvalues of the operator $\hat{\mathbf{k}}$. $\mathbf{k}$ is called the *wave vector* and is used to label irreps of the lattice group. $\mathbf{k}$ can be expressed as

$$\mathbf{k} = p_1\mathbf{b}_1 + p_2\mathbf{b}_2 + p_3\mathbf{b}_3 . \tag{10-47}$$

One of the solutions of (10-46) is easily found to be

$$\psi_{\mathbf{k}}(r) = \exp(i\mathbf{k}\cdot\mathbf{r}) = \exp[2\pi i(p_1\xi_1 + p_2\xi_2 + p_3\xi_3)] . \tag{10-48a}$$

Since $\exp(i\mathbf{K}_m\cdot\mathbf{R}_n) = 1$ from (10-41a), $\psi_{\mathbf{k}+\mathbf{K}_m} = \exp(i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r})$ is also a solution of (10-46). Therefore the irreps $\mathbf{k}$ and $\mathbf{k}+\mathbf{K}_m$ of the lattice group are equivalent and $\mathbf{k}$ and $\mathbf{k}+\mathbf{K}_m$ are referred to as equivalent wave vectors, denoted by

$$\mathbf{k} \doteq \mathbf{k} + \mathbf{K}_m . \tag{10-48b}$$

The most general form of the basis belonging to the irrep $\mathbf{k}$ of the lattice group is

$$\varphi^{(\mathbf{k})}(\mathbf{r}) = \sum_{\mathbf{K}_m} V(\mathbf{k}+\mathbf{K}_m)\exp[i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}] , \tag{10-48c}$$

where $V(\mathbf{k}+\mathbf{K}_m)$ are coefficients.

According to (3-348), the projection operator for the lattice group is

$$P^{(\mathbf{k})} = \text{const.}\sum_{\mathbf{R}_n}\exp[i(\mathbf{k}-\hat{\mathbf{k}})\cdot\mathbf{R}_n] . \tag{10-49}$$

The CSCO of the lattice group can be conveniently chosen as the momentum operator

$$\hat{\mathbf{k}} = -i\nabla \tag{10-45b}$$

with the eigenvalue $\mathbf{k}$ modulo $\mathbf{K}_m$.

10.9. The Brillouin Zone

On the basis of the above discussion, it follows that we can obtain all the irreps of the lattice group by allowing the components p_1, p_2 and p_3 of the wave vector $\mathbf{k}$ to range over a unit interval.

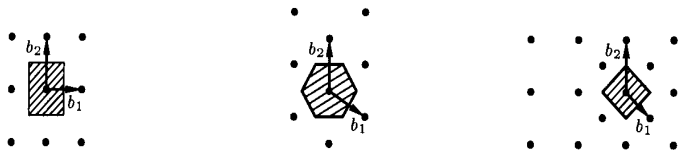
To visualize the region of space in which $\mathbf{k}$ must lie, let us introduce the primitive cell for the reciprocal lattice, which is defined, as in the case for the space lattice, as the parallelepiped formed by the basis vectors $\mathbf{b}_1, \mathbf{b}_2$ and $\mathbf{b}_3$. The primitive cell defined in this way, though simple, has the disadvantage that it does not exhibit the point-group symmetry of the reciprocal lattice. It is preferable to use the symmetrized primitive cell, known as the *Wigner–Seitz cell*, which is defined as the region bounded by the planes bisecting normally the vectors joining reciprocal lattice points. This region surrounding the origin is called the *Brillouin zone* or the first Brillouin zone. We thus conclude that to obtain all the inequivalent irreps of the lattice group, one only needs to let the wave vector $\mathbf{k}$ runs over all the points in the Brillouin zone.

The vector $\mathbf{k}$ in the Brillouin zone is called the *reduced wave vector*. Therefore, an irrep of the lattice group is labelled by a point in the Brillouin zone, or by a reduced wave vector $\mathbf{k}$. Some examples of Brillouin zones for two-dimensional lattices are shown in Fig. 10.9. The Brillouin zones or the Wigner–Seitz cells for a number of three-dimensional lattices can be found in Bradley (1972, Figs. 3.2–3.15), or Slater (1962).

The points in a Brillouin zone are divided into two groups.

1. General points: A wave vector $\mathbf{k}$ is called a general point if it does not have any symmetry, that is, for any operator $\alpha \in \mathbf{G}_0$, $\alpha\mathbf{k}$ and $\mathbf{k}$ are not equivalent.

2. Special points: A point with a certain kind of symmetry is called a special point. For example, the point that lies on a rotation axis or a reflection plane and therefore is invariant under the rotation or reflection, or the point $\mathbf{k}$ in a surface of the Brillouin zone which may be invariant or goes to its equivalent $\mathbf{k}' = \mathbf{k} + \mathbf{K}_m$ under a rotation or reflection.



Simple rectangular Hexagonal Face-centered square

Fig. 10.9. The Brillouin zones for two-dimensional lattices [taken from Elliott (1979)].

Special points are subdivided into two groups (Bradley 1972).

1. Points of symmetry: $\mathbf{k}$ is called a point of symmetry if there exists a neighborhood of $\mathbf{k}$ in which $\mathbf{k}$ is the point with the highest symmetry.

2. Lines or planes of symmetry: $\mathbf{k}$ is called a line (plane) of symmetry if in a sufficiently small neighborhood of $\mathbf{k}$ there is always a line (plane) through $\mathbf{k}$, all points of which have the same symmetry as that of $\mathbf{k}$.

The special points in a Brillouin zone are labelled by the standard solid state physics symbols, for example Γ, X, or M (see Bradley 1972, pp. 96–118).

Of all the rotations in the point group $\mathbf{P}$, those which leave the wave vector $\mathbf{k}$ invariant modulo a reciprocal lattice vector form a subgroup of $\mathbf{P}$ designated by $\mathbf{P}(\mathbf{k})$:

$$\mathbf{P}(\mathbf{k}) = \{\alpha \in \mathbf{P} : \alpha\mathbf{k} \doteq \mathbf{k}\} . \tag{10-50}$$

$\mathbf{P}(\mathbf{k})$ is referred to as the symmetry group of the wave vector $\mathbf{k}$. The symmetry groups $\mathbf{P}(\mathbf{k})$ are listed in Bradley (1972, Table 3.6). Examples are given in Sec. 10.16.

10.10. The Electron State in a Periodic Potential

Consider an electron moving in a crystal. As a first approximation, we can use the independent particle model which assumes that each electron moves independently in a fixed averaged potential $V(\mathbf{r})$, where the potential has the translation symmetry $V(\mathbf{r} + \mathbf{R}_n) = V(\mathbf{r})$. If the crystal does not have symmetries other than the translational symmetry, then the lattice group is the symmetry group of the electron Hamiltonian, and the electron eigenstates must belong to an irrep $\mathbf{k}$ of the lattice group. We know that $\exp(i\mathbf{k}\cdot\mathbf{r})$ is a basis vector of the irrep $\mathbf{k}$. Suppose $w_{\mathbf{k}}(\mathbf{r})$ is a basis vector for the identity rep of the lattice group

$$\{\varepsilon|R_n\}w_{\mathbf{k}}(\mathbf{r}) = w_{\mathbf{k}}(\mathbf{r} - \mathbf{R}_n) = w_{\mathbf{k}}(\mathbf{r}) , \tag{10-51a}$$

then the general expression for the basis vector of the irrep $\mathbf{k}$ is

$$\varphi^{(k)}(\mathbf{r}) = w_{\mathbf{k}}(\mathbf{r}) \exp(i\mathbf{k}\cdot\mathbf{r}) . \tag{10-51b}$$

The wave function $\varphi^{(\mathbf{k})}(\mathbf{r})$ for an electron in a crystal is called the *Bloch function.* The function $w_k(\mathbf{r})$ is found from the Schrödinger equation

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + V(\mathbf{r})\right]\varphi^{(\mathbf{k})}(\mathbf{r}) = \varepsilon(\mathbf{k})\varphi^{(k)}(\mathbf{r}) , \tag{10-52a}$$

or

$$\left[\frac{\hbar^2}{2M}(\nabla + i\mathbf{k})^2 + \varepsilon(\mathbf{k}) - V(\mathbf{r})\right] w_{\mathbf{k}}(\mathbf{r}) = 0 . \tag{10-52b}$$

Since $w_k(\mathbf{r})$ is a periodic function of $\mathbf{r}$, this differential equation needs to be solved only within a single cell, using the periodic boundary conditions on $w_{\mathbf{k}}(\mathbf{r})$ at the edge of the cell. Group theory has thus enabled us to replace a problem for the whole crystal by one for a single cell.

The periodic function $w_{\mathbf{k}}(\mathbf{r})$ can be expanded into the Fourier series

$$w_k(\mathbf{r}) = \sum_{\mathbf{K}_m} v(\mathbf{k} + \mathbf{K}_m) \exp[i\mathbf{K}_m \cdot \mathbf{r}] . \tag{10-53}$$

We see, by inserting (10-53) into (10-51b), that (10-48c) is another expression for the Bloch function.

10.11. Representation Space of the Space Group

Since the translation group $\mathbf{T}$ is a subgroup of the space group $\mathbf{G}$, naturally we shall choose the group chain $\mathbf{G} \supset \mathbf{T}$ to classify the irreducible bases of $\mathbf{G}$. From (10-48b) we know that

$$\psi_{\mathbf{k}} = \exp[i(\mathbf{k} + \mathbf{K}_m)\cdot\mathbf{r}] \tag{10-54a}$$

carries the irrep $\mathbf{k}$ of $\mathbf{T}$, with $\mathbf{k}$ restricted to the Brillouin zone. The functions of (10-54a) with the same $\mathbf{k}$ but all possible $\mathbf{K}_m$ form an eigenspace $\mathcal{L}_{\mathbf{k}}$ of the translation operator $\{\varepsilon|\mathbf{R}_n\}$,

$$\mathcal{L}_{\mathbf{k}} = \{\exp[i(\mathbf{k} + \mathbf{K}_m)\cdot\mathbf{r}_m] : \mathbf{K}_m \in L^{-1}\} . \tag{10-54b}$$

Our primary task is to find linear combinations of (10-54a) with $\mathbf{k}$ and $\mathbf{K}_m$ such that the combinations form the irreducible bases of the space group $\mathbf{G}$. As a routine procedure, we apply all the group elements of $\mathbf{G}$ to the function $\psi_{\mathbf{k}}$ and pick out the linearly independent functions that will carry a rep of $\mathbf{G}$, and then reduce this rep into irreps of $\mathbf{G}$. From (10-33) and (10-54a),

$$\{\alpha|\mathbf{a}\}\psi_{\mathbf{k}} = \exp[-i\alpha(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{a}]\exp[i\alpha(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}] \ . \tag{10-55a}$$

It is seen that the translation part $\{\varepsilon|\mathbf{a}\}$ of the group element $\{\alpha|\mathbf{a}\}$ only affects the phase factor, whereas the rotation part α changes the wave vector $\mathbf{k}+\mathbf{K}_m$ into $\alpha(\mathbf{k}+\mathbf{K}_m)$. Therefore, $\{\alpha|\mathbf{a}\}\psi_{\mathbf{k}}$ belongs to the eigenspace $\mathcal{L}_{a\mathbf{k}}$ of $\{\varepsilon|\mathbf{R}_n\}$. Equation (10-55a) shows that the functions $\{\alpha|\mathbf{V}(\alpha)+\mathbf{R}_n\}\psi_{\mathbf{k}}$ with the same α but different $\mathbf{R}_n$ are linearly dependent. Consequently, although the space group $\mathbf{G}$ has an infinite number of elements, it generates from ψ_k only $|\mathbf{G}_0|$ linearly independent functions, which can be chosen as

$$\begin{aligned}\psi_{a_j\mathbf{k}} &= \{\alpha_j|\mathbf{V}(\alpha_j)\}\psi_{\mathbf{k}} \\ &= \exp[i\alpha_j(\mathbf{k}+\mathbf{K}_m)\cdot(\mathbf{r}-\mathbf{V}(\alpha_j)] \ , \quad j=1,2,\ldots,|\mathbf{G}_0| \ .\end{aligned} \tag{10-55b}$$

These functions form a rep space

$$\mathcal{L}(*\mathbf{k}) = \{\psi_{a_i k}: \quad i=1,2,\ldots,|\mathbf{G}_0|\} \tag{10-55c}$$

for the space group $\mathbf{G}$. In general $\mathcal{L}(*k)$ is a reducible space of $\mathbf{G}$.

Stated differently, in a rep space with Bloch functions as basis vectors, the space group $\mathbf{G}$ has only $|\mathbf{G}_0|$ linearly independent operators $\{\alpha_i|\mathbf{V}(\alpha_i)\}$, which form a rep space

$$L(*\mathbf{k}) = \{\{\alpha_i|\mathbf{V}(\alpha_i)\}: \quad i=1,2,\ldots,|\mathbf{G}_0|\} \tag{10-55d}$$

for the space group $\mathbf{G}$. The spaces $\mathcal{L}(*\mathbf{k})$ and $L(*\mathbf{k})$ are isomorphic.

10.12. The Little Group G(k)

The problem we face now is how to reduce this $|\mathbf{G}_0|$-dimensional rep of $\mathbf{G}$. According to the procedure introduced in Chapter 3 we need first to find the CSCO of the space group, and then to find the eigenvectors of the CSCO in the space $\mathcal{L}(*\mathbf{k})$. However, this procedure proves to be unsuitable, since the class operator of the space group has a rather complicated structure. We have to resort to another strategy. We first sandwich a group $\mathbf{H}$ between the space group $\mathbf{G}$ and the translation group $\mathbf{T}$; then we determine the $\mathbf{H}\supset\mathbf{T}$ irreducible basis, and finally we get the $\mathbf{G}\supset\mathbf{H}\supset\mathbf{T}$ irreducible basis.

Of the $|\mathbf{G}_0|$ operations in the point group $\mathbf{G}_0$, all the rotations γ which leave the wave vector $\mathbf{k}$ invariant modulo a reciprocal lattice vector, that is,

$$\gamma\mathbf{k} = \mathbf{k}+\mathbf{K}_m \doteq \mathbf{k} \ , \tag{10-56}$$

form a subgroup of $\mathbf{G}_0$ denoted

$$\mathbf{G}_0(\mathbf{k}) = \{\gamma\in\mathbf{G}_0 : \gamma\mathbf{k}\doteq\mathbf{k}\} \ . \tag{10-57a}$$

$\mathbf{G}_0(\mathbf{k})$ is called the *little co-group* .

The little co-group $\mathbf{G}_0(\mathbf{k})$ is the intersection of the symmetry group $\mathbf{P}(\mathbf{k})$ of $\mathbf{k}$ and the isogonal point group $\mathbf{G}_0$,

$$\mathbf{G}_0(\mathbf{k}) = \mathbf{P}(\mathbf{k})\cap\mathbf{G}_0 \ . \tag{10-57b}$$

All the elements $\{\gamma|\mathbf{V}(\gamma)+\mathbf{R}_n\}$, for $\gamma \in \mathbf{G}_0(\mathbf{k})$ and $\mathbf{R}_n \in L$, form another space group designated as

$$\mathbf{G}(\mathbf{k}) = \{\{\gamma_i|\mathbf{V}(\gamma_i)+\mathbf{R}_n\}: \quad i=1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|, \mathbf{R}_n \in L\} \,. \tag{10-58}$$

$\mathbf{G}(\mathbf{k})$ is referred to as the *little group* , or the *group of the wave vector* $\mathbf{k}$. $\mathbf{G}(\mathbf{k})$ is a subgroup of $\mathbf{G}$ and contains $\mathbf{T}$ as its subgroup. Therefore, the subgroup $\mathbf{G}(\mathbf{k})$ is a candidate for the group $\mathbf{H}$ to be sandwiched between $\mathbf{G}$ and $\mathbf{T}$. Another way of saying this is that for any subgroup $\mathbf{H}$ of the space group $\mathbf{G}$, the point group of $\mathbf{H}$ must be the symmetry group of a certain wave vector $\mathbf{k}$. Thus we can use the wave vector $\mathbf{k}$ to label this subgroup, that is, use $\mathbf{G}(\mathbf{k})$ to denote $\mathbf{H}$.

The order of $\mathbf{G}_0(\mathbf{k})$ is a divisor of the order of $\mathbf{G}_0$,

$$q = |\mathbf{G}_0|/|\mathbf{G}_0(\mathbf{k})| \,, \tag{10-59}$$

where q is an integer.

The $|\mathbf{G}_0(\mathbf{k})|$ linearly independent functions

$$\psi_{\gamma_i\mathbf{k}} = \{\gamma_i|\mathbf{V}(\gamma_i)\}\psi_{\mathbf{k}} \tag{10-60a}$$

form a space

$$\mathcal{L}(\mathbf{k}) = \{\psi_{\gamma_i\mathbf{k}}: \quad i=1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|\} \,. \tag{10-60b}$$

$\mathcal{L}(\mathbf{k})$ is a subspace of $\mathcal{L}_{\mathbf{k}}$ as well as a subspace of $\mathcal{L}(*\mathbf{k})$, and is a $|\mathbf{G}_0(\mathbf{k})|$-dimensional rep space of the little group $\mathbf{G}(\mathbf{k})$. $\mathcal{L}(\mathbf{k})$ is in general reducible. By decomposing $\mathcal{L}(\mathbf{k})$, we can get the $\mathbf{G}(\mathbf{k}) \supset \mathbf{T}$ irreducible basis.

Since $\mathcal{L}(\mathbf{k})$ is an eigenspace of $\{\varepsilon|\mathbf{R}_n\}$, in $\mathcal{L}(\mathbf{k})$ we have

$$\{\varepsilon|\mathbf{R}_n\} = \exp(-i\mathbf{k}\cdot\mathbf{R}_n)\mathbf{I} \,, \tag{10-61}$$

where $\mathbf{I}$ is a unit matrix. Therefore, in the space $\mathcal{L}(\mathbf{k})$, the translation operator $\{\varepsilon|\mathbf{R}_n\}$ commutes with any operator of $\mathbf{G}(\mathbf{k})$.

10.13. The Representation Groups $\mathbf{G}_{\mathbf{k}}$ and $\mathbf{G}'_{\mathbf{k}}$

10.13.1. The rep group $\mathbf{G}_{\mathbf{k}}$

From

$$\{\gamma_j|\mathbf{V}(\gamma_j)+\mathbf{R}_n\} = \{\varepsilon|\mathbf{R}_n\}\{\gamma|\mathbf{V}(\gamma_j)\} \tag{10-62a}$$

and Eq. (10-61), we can see that the group operators of $\mathbf{G}(\mathbf{k})$ in the space $\mathcal{L}(\mathbf{k})$ are related by

$$\{\gamma_j|\mathbf{V}(\gamma_j)+\mathbf{R}_n\} = \varepsilon(j,n)\{\gamma_j|\mathbf{V}(\gamma_j)\} \,, \tag{10-62b}$$

$$\varepsilon(j,n) = \varepsilon(n) = \exp(-i\mathbf{k}\cdot\mathbf{R}_n) \,. \tag{10-62c}$$

To avoid notational clumsiness, we use the symbol $\{\gamma|\mathbf{V}(\gamma)\}$ to denote both the group element and the corresponding operator or representative matrix in $\mathcal{L}(\mathbf{k})$.

Equation (10-62b) shows that in the rep space $\mathcal{L}(\mathbf{k})$ the little group $\mathbf{G}(\mathbf{k})$ has only $|\mathbf{G}_0(\mathbf{k})|$ linearly independent operators $\{\gamma_i|\mathbf{V}(\gamma_i)\}, i=1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|$.

Using (10-24), (10-25b) and (10-62b) we obtain the multiplication relation for these independent operators,

$$\{\gamma_i|\mathbf{V}(\gamma_i)\}\{\gamma_j|\mathbf{V}(\gamma_j)\} = \mu(i,j)\{\gamma_{ij}|\mathbf{V}(\gamma_{ij})\} \,, \tag{10-63a}$$

$$\mu(i,j) = \exp(-i\mathbf{k}\cdot\mathbf{R}_{ij})$$
$$= \exp\{-i\mathbf{k}\cdot[\mathbf{V}(\gamma_i) + \gamma_i\mathbf{V}(\gamma_j) - \mathbf{V}(\gamma_{ij})]\} \ . \tag{10-63b}$$

By identifying $\mathcal{L}(\mathbf{k}), |\mathbf{G}_0(\mathbf{k})|, \{\gamma_i|\mathbf{V}(\gamma_i)\}$, and $\mu(i,j)$ with $L, |\mathbf{g}|, R_i$, and $\eta(i,j)$, respectively, in Sec. 8.12 we see that all the distinct operators $\varepsilon(i,n)\{\gamma_i|\mathbf{V}(\gamma_i)\}$ form a rep group [compare with Eq. (8-138c)],

$$\mathbf{G}_\mathbf{k} = \{\{\gamma_i|V(\gamma_i)\}: \quad i = 1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|\}_m \ , \tag{10-63c}$$

where m is an integer depending on $\mathbf{k}$ (see the discussion below).

The rep group $\mathbf{G}_k$ can be regarded as a faithful rep of an abstract group $\widehat{\mathbf{G}}_\mathbf{k}$. The abstract group could be, for example, the so–called central extension $\overline{\mathbf{G}}^{\mathbf{k}*}$ defined by Schur (see Bradley 1972). Notice that what is called the representation group by Birman (1974) is just another name for the central extension, and thus differs from our definition for the rep group.

From (10-62b) it is clear that the irreducible basis of the little group $\mathbf{G}(\mathbf{k})$ in the space $\mathcal{L}(\mathbf{k})$ is identical to that of the rep group $\mathbf{G}_\mathbf{k}$; their representation matrices are related by

$$D^{(\mathbf{k})(\nu)}(\{\gamma|\mathbf{V}(\gamma) + \mathbf{R}_n\}) = \exp(-i\mathbf{k}\cdot\mathbf{R}_n)D^{(\mathbf{k})(\nu)}(\{\gamma|\mathbf{V}(\gamma)\}) \ , \tag{10-64}$$

where $(\mathbf{k})(\nu)$ is the label for the irrep of $\mathbf{G}(\mathbf{k})$ or $\mathbf{G}_\mathbf{k}$. It is to be noted that we always regard the symbol $D^{(j)}(X)$ as the representative matrix of an operator X with respect to a certain basis labelled by the index j, and $D^{(j)}(Y)$ is the representation matrix for another operator Y, while X and Y may belong to *different* groups. This notation is consistent with the convention used in quantum mechanics and is very convenient. The irrep $D^{(\mathbf{k})(\nu)}(\{\gamma|\mathbf{c}\})$ is called the small rep of the little group $\mathbf{G}(\mathbf{k})$.

If the wave vector $\mathbf{k}$ is a point of symmetry, then $\mathbf{k}$ is of the form

$$\mathbf{k} = \frac{1}{m}(m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3) \ , \tag{10-65a}$$

where m and m_i are integers. In such a case, the phase factor $\mu(i,j)$ in (10-63b) is of the form

$$\mu(i,j) = \exp(-i\mathbf{k}\cdot\mathbf{R}_{ij}) = \exp(2\pi li/m) \ , \quad l = 0,1,\ldots m-1 \ . \tag{10-65b}$$

Hence the rep group $\mathbf{G}_\mathbf{k}$ is an *m–fold covering group of* $\mathbf{G}_0(\mathbf{k})$ with the elements

$$\exp(2\pi li/m)\{\gamma_j|\mathbf{V}(\gamma_j)\} \ , \quad j = 1,2,\ldots,|\mathbf{G}_0(\mathbf{k})| \ , \quad l = 0,1,\ldots,m-1 \ . \tag{10-65c}$$

Nevertheless, if $\mathbf{k}$ is a line (or plane) of symmetry, for instance if $\mathbf{k}$ is of the form

$$\mathbf{k} = \frac{1}{m'}(m_1\mathbf{b}_1 + m_2\mathbf{b}_2) + p_3\mathbf{b}_3 \ , \tag{10-65d}$$

where p_3 is an arbitrary number, say an irrational number, then the phase factor $\mu(i,j)$ will not have the simple form of (10-65b). It is thus seen that the factor system μ has the unpleasant feature that the integer $m = |\mathbf{G}_\mathbf{k}|/|\mathbf{G}_0(\mathbf{k})|$ depends on the wave vector $\mathbf{k}$ and may become very large for $\mathbf{k}$ in a line (or plane) of symmetry. We address this problem in the next subsection.

10.13.2. The rep group $\mathbf{G}'_{\mathbf{k}}$

Let us apply the following gauge transformation to the group elements of $\mathbf{G}(\mathbf{k})$:

$$\begin{aligned} R_i &\equiv \{\gamma_i|\mathbf{V}(\gamma_i)\}' \\ &= \exp[i\mathbf{k}\cdot\mathbf{V}(\gamma_i)]\{\gamma_i|\mathbf{V}(\gamma_i)\} \ . \end{aligned} \tag{10-66}$$

It follows from (10-63a) that in the space $\mathcal{L}(\mathbf{k})$ we have

$$R_iR_j = \eta(i,j)R_{ij} \ , \tag{10-67a}$$

$$\eta(i,j) = \exp\{-i\mathbf{k}\cdot[\gamma_i\mathbf{V}(\gamma_j) - \mathbf{V}(\gamma_j)]\} \ . \tag{10-67b}$$

According to Eq. (10-56a)

$$\gamma_i^{-1}\mathbf{k} = \mathbf{k} + \mathbf{K}_{\gamma_i} \ , \tag{10-67c}$$

where $\mathbf{K}_{\gamma_i}$ is a reciprocal lattice vector. Thus

$$\eta(i,j) = \exp[-i\mathbf{K}_{\gamma_i}\cdot\mathbf{V}(\gamma_j)] \ . \tag{10-67d}$$

With Eqs. (10-23) and (10-67d), the phase factor $\eta(j,k)$ is of the form

$$\eta(j,k) = \exp(2\pi i a_{jk}/m) \ , \quad m = 2,3,4,6 \ , \tag{10-68}$$

where a_{jk} is an integer depending on j and k. Therefore, in the space $\mathcal{L}(\mathbf{k})$, the $m|\mathbf{G}_0(\mathbf{k})|$ operators

$$R_j^{(l)} = \exp(2\pi l i/m)R_j \ , \quad j = 1,2,\ldots,|\mathbf{G}_0(\mathbf{k})| \ , \quad l = 0,1,\ldots,m-1 \ , \tag{10-69}$$

form a rep group designated as

$$\mathbf{G}'_k = \{R_i : i = 1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|\}_m \ . \tag{10-70}$$

The rep group $\mathbf{G}'_{\mathbf{k}}$ is an m–fold covering group of the point group $\mathbf{G}_0(\mathbf{k})$ where the integer m depends only on what kind of fractional translation the space group $\mathbf{G}$ has and takes only four possible values, 2, 3, 4 and 6, for all 230 space groups.

Since R_i differs from $\{\gamma_i|\mathbf{V}(\gamma_i)\}$ only by the phase factor $\exp[i\mathbf{k}\cdot\mathbf{V}(\gamma_i)]$, the groups $\mathbf{G}'_{\mathbf{k}}$, $\mathbf{G}_{\mathbf{k}}$, and $\mathbf{G}(\mathbf{k})$ have identical irreducible bases, and their matrices, upon using (10-64) and (10-66), are related to one another by

$$D^{(\mathbf{k})(\nu)}(\{\gamma_i|\mathbf{V}(\gamma_i)\}) = \exp(-i\mathbf{k}\cdot\mathbf{V}(\gamma_i))D^{(\mathbf{k})(\nu)}(R_i) \ , \tag{10-71a}$$

$$D^{(\mathbf{k})(\nu)}(\{\gamma_i|\mathbf{c}_i\}) = \exp(-i\mathbf{k}\cdot\mathbf{c}_i)D^{(\mathbf{k})(\nu)}(R_i) \ , \tag{10-71b}$$

where $D^{(\mathbf{k})(\nu)}(R_i)$ is the irreducible matrix for the element R_i of the rep group $\mathbf{G}'_k$.

For notational convenience, we often use $\Delta(\gamma_i)$ to denote the matrix $D^{(\mathbf{k})(\nu)}(R_i)$, that is,

$$\Delta(\gamma_i) \equiv D^{(\mathbf{k})(\nu)}(R_i) = D^{(\mathbf{k})(\nu)}(\{\gamma_i|\mathbf{V}(\gamma_i)\}') \ . \tag{10-72a}$$

Equation (10-71b) then reads

$$D^{(\mathbf{k})(\nu)}(\{\gamma_i|\mathbf{c}_i\}) = \exp(-i\mathbf{k}\cdot\mathbf{c}_i)\Delta(\gamma_i) \ . \tag{10-71c}$$

It follows from (10-67a) and (10-72a), that

$$\Delta(\gamma_i)\Delta(\gamma_j) \equiv \eta(i,j)\Delta(\gamma_i\gamma_j) \ . \tag{10-72b}$$

Δ is the projective irrep of the point group $\mathbf{G}_0(\mathbf{k})$.

In summary, the problem of finding the irreps of an infinite group $\mathbf{G}(\mathbf{k})$ is converted into finding that of the rep group $\mathbf{G}_k$ or $\mathbf{G}'_\mathbf{k}$. For those wave vectors $\mathbf{k}$ which are lines or planes of symmetry, we must work with the rep group $\mathbf{G}'_\mathbf{k}$, while for those $\mathbf{k}$ which are points of symmetry, we can work with either the group $\mathbf{G}_\mathbf{k}$ or with $\mathbf{G}'_\mathbf{k}$. However, the multiplication relation (10-67a) for $\mathbf{G}'_\mathbf{k}$ is much simpler than that for $\mathbf{G}_\mathbf{k}$; in the following we shall work only with the rep group $\mathbf{G}'_\mathbf{k}$, irrespective of points of symmetry or line (planes) of symmetry.

The $|\mathbf{G}_0(\mathbf{k})|$ functions

$$\psi_j \equiv R_j \exp[i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}] \ , \quad j = 1,2,\ldots,|\mathbf{G}_0(\mathbf{k})| \ , \tag{10-73a}$$

carry the rep space $\mathcal{L}(\mathbf{k})$ for $\mathbf{G}'_\mathbf{k}$, which coincides with the space $\mathcal{L}(\mathbf{k})$ of (10-60b). The group space of the rep group $\mathbf{G}'_\mathbf{k}$ is denoted by

$$L(\mathbf{k}) = \{R_i : \quad i = 1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|\} \ . \tag{10-73b}$$

The spaces $\mathcal{L}(\mathbf{k})$ and $L(\mathbf{k})$ are isomorphic, and it is more convenient to work with the latter. In the following we work mainly with $L(\mathbf{k})$.

10.13.3. Special cases of the rep group $\mathbf{G}'_\mathbf{k}$

The following four cases need to be considered separately.

1. For a general $\mathbf{k}$ point. This is a trivial case, since now $\mathbf{G}'_\mathbf{k} = \mathbf{G}_\mathbf{k} = \{\varepsilon\}$.

2. For the symmorphic space group, or the non-symmorphic space group whose little group $\mathbf{G}(\mathbf{k})$ is symmorphic for the wave vector $\mathbf{k}$ under consideration. For these cases, $\mathbf{V}(\gamma) \equiv 0$, and according to (10-63b) and (10-67d), the phase factor $\mu(i,j) = \eta(i,j) = 1$, hence

$$\mathbf{G}_\mathbf{k} = \mathbf{G}'_\mathbf{k} = \mathbf{G}_0(\mathbf{k}) \ , \tag{10-74}$$

that is, the rep group $\mathbf{G}'_\mathbf{k}$ (or $\mathbf{G}_\mathbf{k}$) is identical to the point group $\mathbf{G}_0(\mathbf{k})$, whose irreps are already known. In passing we point out that in such cases the space $L(\mathbf{k}) = \{R_i\} = \{\gamma_i\}$ is the regular rep space of the point group $\mathbf{G}_0(\mathbf{k})$.

3. For an interior point of a Brillouin zone. When the wave vector $\mathbf{k}$ is not on the surface of the Brillouin zone, the only possibility for $\gamma\mathbf{k} = \mathbf{k} + \mathbf{K}_m$ is that $\mathbf{K}_m = 0$ so that

$$\gamma\mathbf{k} = \mathbf{k} \ . \tag{10-75}$$

Comparing this with (10-67c), we see that now $\mathbf{K}_\gamma \equiv 0$, and the phase factor in (10-67a) is again equal to one, $\eta(i,j) \equiv 1$. Therefore, the rep group $\mathbf{G}'_\mathbf{k}$ is isomorphic to the point group $\mathbf{G}_0(\mathbf{k}) = \{\gamma_i\}$. Suppose $D^{(\nu)}$ is the irrep of the point group $\mathbf{G}_0(\mathbf{k})$. Then the irrep of the rep group $\mathbf{G}'_\mathbf{k}$ is

$$D^{(\mathbf{k})(\nu)}(R_i) = D^{(\nu)}(\gamma_i) \ , \tag{10-76a}$$

while the irrep of the little group $\mathbf{G}(\mathbf{k})$ is [Eq. (10-71b)],

$$D^{(\mathbf{k})(\nu)}(\{\gamma|\mathbf{c}\}) = \exp(-i\mathbf{k}\cdot\mathbf{c})D^{(\nu)}(\gamma) \ . \tag{10-76b}$$

Observe that, for the origin point $\mathbf{k} = 0$, we again have

$$\mathbf{G}_\mathbf{k} = \mathbf{G}'_\mathbf{k} \ , \tag{10-77}$$

and again the distinction between $\mathbf{G}_\mathbf{k}$ and $\mathbf{G}'_\mathbf{k}$ disappears.

It should also be noted that for the case of interior points, although the rep group $\mathbf{G}'_{\mathbf{k}}$ and the point group $\mathbf{G}_0(\mathbf{k})$ have identical irreps (10-76a), their irreducible bases do not coincide. For example, if

$$\varphi^{(\nu)}_{\mathbf{k},a} = \sum_i u^{(\nu)}_{a,i} \gamma_i \psi_{\mathbf{k}} \tag{10-78a}$$

is the irreducible basis of $\mathbf{G}_0(\mathbf{k})$, where $u^{(\nu)}_{a,i}$ are coefficients and $\psi_{\mathbf{k}} = \exp[i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}]$, then the corresponding irreducible basis of $\mathbf{G}'_{\mathbf{k}}$ is

$$\psi^{(\nu)}_{\mathbf{k},a} = \sum_i u^{(\nu)}_{a,i} \{\gamma_i | \mathbf{V}(\gamma_i)\}' \psi_{\mathbf{k}} \ . \tag{10-78b}$$

4. For a point on the surface of a Brillouin zone and for non-symmorphic little groups. For cases (1)–(3) above, the irreps of the rep group $\mathbf{G}'_{\mathbf{k}}$ can be directly taken over from those of the point group $\mathbf{G}_0(\mathbf{k})$. The only case for which the irreps of $\mathbf{G}'_{\mathbf{k}}$ cannot be obtained in this way and have to be worked out anew is when the wave vector $\mathbf{k}$ is on the surface of a Brillouin zone and its little group $\mathbf{G}(\mathbf{k})$ is non-symmorphic.

10.14. The Irreducible Basis and Matrices of $\mathbf{G}'_{\mathbf{k}}$

10.14.1. The group table of $\mathbf{G}'_{\mathbf{k}}$

The group table of $\mathbf{G}'_{\mathbf{k}}$ can easily be constructed from the group table $\gamma_\rho\gamma_\sigma = \gamma_{\rho\sigma}$ of the little co-group $\mathbf{G}_0(\mathbf{k})$ by replacing γ's with R's and multiplying the $(\rho\sigma)$ entry with the phase factor,

$$\eta(\rho,\sigma) = \exp[-i(\gamma_\rho^{-1}\mathbf{k}-\mathbf{k})\cdot\mathbf{V}(\gamma_\sigma)] \ . \tag{10-79a}$$

Since the phase factors $\eta(\rho,\sigma)$ are crucial for the whole process of analysis, we give a simple formula for calculating them. For that purpose we introduce the following notations. Let

$$\begin{aligned} &\mathbf{b} = (\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3) \ , \quad \mathbf{t} = (\mathbf{t}_1,\mathbf{t}_2,\mathbf{t}_3) \ , \\ &\mathbf{p} = (p_1,p_2,p_3) \ , \quad \tau_\sigma = (\tau_{\sigma 1},\tau_{\sigma 2},\tau_{\sigma 3}) \ . \end{aligned} \tag{10-79b}$$

The wave vector $\mathbf{k}$ and the non-primitive translation $\mathbf{V}(\gamma_\sigma)$ can be expressed as

$$\begin{aligned} &\mathbf{k} = \mathbf{p}\cdot\mathbf{b} = p_1\mathbf{b}_1 + p_2\mathbf{b}_2 + p_3\mathbf{b}_3 \ , \\ &\mathbf{V}(\gamma_\sigma) = \tau_\sigma\cdot\mathbf{t} = \tau_{\sigma 1}\mathbf{t}_1 + \tau_{\sigma 2}\mathbf{t}_2 + \tau_{\sigma 3}\mathbf{t}_3 \ . \end{aligned} \tag{10-79c}$$

It can be shown that under rotations (p_1,p_2,p_3) transforms as $(\mathbf{t}_1,\mathbf{t}_2,\mathbf{t}_3)$, whereas $(\tau_{\sigma 1},\tau_{\sigma 2},\tau_{\sigma 3})$ transforms as $(\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3)$, and $\mathbf{k}$ and $\mathbf{V}(\gamma_\sigma)$ are invariants.

Furthermore

$$\begin{aligned} &\gamma_\rho^{-1}\mathbf{k} = \gamma_\rho^{-1}(\mathbf{p}\cdot\mathbf{b}) = \mathbf{p}\cdot(\gamma_\rho^{-1}\mathbf{b}) = \mathbf{p}_\rho\cdot\mathbf{b} \ , \\ &\mathbf{p}_\rho = \gamma_\rho\mathbf{p} = (p_{\rho 1},p_{\rho 2},p_{\rho 3}) \ . \end{aligned} \tag{10-79d}$$

The transformed vector $\mathbf{p}_\rho = \gamma_\rho\mathbf{p}$ can be found from Table 10.21-2 by replacing the $\mathbf{t}_i$'s with $\mathbf{p}_i$'s. Using (10-79a), (10-79b) and (10-79d) we finally obtain

$$\eta(\rho,\sigma) = \exp[-2\pi i(\mathbf{p}_\rho-\mathbf{p})\cdot\tau_\sigma] \ , \tag{10-80a}$$

where

$$(\mathbf{p}_\rho-\mathbf{p})\cdot\tau_\sigma = \sum_{i=1}^{3}(p_{\rho i}-p_i)\tau_{\sigma i} \ . \tag{10-80b}$$

Using the group table of $\mathbf{G}'_{\mathbf{k}}$, one can easily determine the classes of $\mathbf{G}'_{\mathbf{k}}$. The number n of linearly independent class operators of $\mathbf{G}'_{\mathbf{k}}$ is less than the number N of classes, $n < N$. Out of the n linearly independent class operators, we can choose a subset which is a CSCO in the n–dimensional class space of $\mathbf{G}'_{\mathbf{k}}$ and this subset is the CSCO–I of the rep group $\mathbf{G}'_{\mathbf{k}}$. The procedure for finding the CSCO–I and the simple characters of $\mathbf{G}'_{\mathbf{k}}$ is exactly the same as that for an abstract group. An example will be given in Sec. 10.15.

Remark: In Sec. XXI of Chen, Gao & Ma (1985), it was pointed out that "for computer calculations it is expedient to choose self–adjoint CSCO's, since the diagonalization of hermitian matrices is much easier than that of non–hermitian matrices." From experience this observation has been found to be untrue. Indeed the difficulty in finding a self–adjoint CSCO far surpasses that in diagonalizing a non–hermitian CSCO. Therefore it is preferable to choose a linear combination of the class operators, regardless of their being self–adjoint or not, as the CSCO of $\mathbf{G}'_{\mathbf{k}}$.

10.14.2. The CSCO–II and CSCO–III of $\mathbf{G}'_{\mathbf{k}}$

To decompose the group space $L(\mathbf{k})$ of $\mathbf{G}'_{\mathbf{k}}$, we need to introduce a suitable group chain $\mathbf{G}'_{\mathbf{k}} \supset \mathbf{G}'_s$, which can be assumed without loss of generality to be a canonical one. For simplicity we assume $\mathbf{G}'_s$ to be simply a subgroup of $\mathbf{G}'_{\mathbf{k}}$, instead of a subgroup chain, thus

$$\mathbf{G}'_s = \{R_s\} \ , \quad R_s = \{\gamma_s|\mathbf{V}(\gamma_s)\}' \ . \tag{10-81}$$

We also need the intrinsic group $\overline{\mathbf{G}}'_{\mathbf{k}}$ of the rep group $\mathbf{G}'_{\mathbf{k}}$. This is defined by

$$\overline{R}_i R_j = R_j R_i \quad \text{for any} \quad R_j \in L(\mathbf{k}) \ . \tag{10-82}$$

$\overline{\mathbf{G}}'_{\mathbf{k}}$ and $\mathbf{G}'_{\mathbf{k}}$ commute and are anti–isomorphic. Corresponding to the subgroup $\mathbf{G}'_s$ of $\mathbf{G}'_{\mathbf{k}}$ is the intrinsic subgroup

$$\overline{\mathbf{G}}'_s = \{\overline{R}_s\} \tag{10-83}$$

of $\overline{\mathbf{G}}'_{\mathbf{k}}$. Let C and $C(s)$ be the CSCO of $\mathbf{G}'_{\mathbf{k}}$ and $\mathbf{G}'_s$ respectively; then $\overline{C}$ and $\overline{C}(s)$ are the CSCO of $\overline{\mathbf{G}}'_{\mathbf{k}}$ and $\overline{\mathbf{G}}'_s$, respectively, where $\overline{C}$ and $\overline{C}(s)$ are obtained from C and $C(s)$ by replacing the elements of $\mathbf{G}'_{\mathbf{k}}$ with the corresponding intrinsic group elements. Furthermore, we still have $\overline{\overline{C}} = C$.

If $K = (C, C(s), \overline{C}(s))$ is a CSCO in the $|\mathbf{G}_0(\mathbf{k})|$–dimensional space $L(\mathbf{k})$, then K is the CSCO–III of $\mathbf{G}'_{\mathbf{k}}$, while $M = (C, C(s))$ is the CSCO–II of $\mathbf{G}'_{\mathbf{k}}$.

The intrinsic group $\overline{\mathbf{G}}(\mathbf{k})$ of the little group $\mathbf{G}(\mathbf{k})$ is defined by

$$\overline{\mathbf{G}}(\mathbf{k}) = \{\overline{\{\gamma_i|\mathbf{V}(\gamma_i) + \mathbf{R}_n\}} : \quad i = 1, 2, \ldots, |\mathbf{G}_0(\mathbf{k})|, \mathbf{R}_n \in L\} \tag{10-84a}$$

with

$$\overline{\{\gamma_i|\mathbf{c}\}} = \exp(-i\mathbf{k}\bullet\mathbf{c})\overline{R}_i \ , \quad \mathbf{c} = \mathbf{V}(\gamma_i) + \mathbf{R}_n \ . \tag{10-84b}$$

The eigenvector of the CSCO–III of $\mathbf{G}'_{\mathbf{k}}$ in the space $L(\mathbf{k})$ is denoted by $P_a^{(\mathbf{k})(\nu)b}$. Eq. (3-169a) now reads

$$\begin{pmatrix} C \\ C(s) \\ \overline{C}(s) \end{pmatrix} P_a^{(\mathbf{k})(\nu)b} = \begin{pmatrix} \nu \\ a \\ b \end{pmatrix} P_a^{(\mathbf{k})(\nu)b}, \quad a, b = a_1, a_2, \ldots, a_{h_\nu} \ . \tag{10-85}$$

The eigenvector $P_a^{(\mathbf{k})(\nu)b}$ is a linear combination of R_i,

$$P_a^{(\mathbf{k})(\nu)b} = \sum_{i=1}^{|G_0(\mathbf{k})|} u_{ab,i}^{(\mathbf{k})(\nu)} R_i \ . \tag{10-86}$$

Equations (3-173), (3-176) and (3-180) still hold under the substitutions

$$g \to |\mathbf{G}_0(\mathbf{k})| \ , \quad N \to n \ , \quad u_{\nu mk,a} \to u^{(\mathbf{k})(\nu)}_{ab,i} \ . \tag{10-87}$$

Then the coefficients $u^{(\mathbf{k})(\nu)}_{ab,i}$ are the solutions to (3-176).

The eigenvector $P^{(\mathbf{k})(\nu)b}_a$, for $a,b = a_1,\ldots,a_{h_\nu}$, constitutes the $\mathbf{G}'_\mathbf{k} \supset \mathbf{G}'_s$ and $\overline{\mathbf{G}}'_\mathbf{k} \supset \overline{\mathbf{G}}'_s$ irreducible basis. Eq. (3-173) shows that the number of times that the irrep $(\mathbf{k})(\nu)$ of $\mathbf{G}'_\mathbf{k}$ appears in the space $L(\mathbf{k})$ is equal to its dimension h_ν.

One of the advantages of the EFM for constructing the irreducible basis or irreps of $\mathbf{G}(\mathbf{k})$ is that the subgroup chain used to classify the irreducible basis or irrep can be chosen at will without the restriction that the subgroup has to be an invariant subgroup of $\mathbf{G}(\mathbf{k})$.

However, if for some circumstances we are only interested in obtaining irreps of $\mathbf{G}(\mathbf{k})$ without the requirement that they be in a certain classification scheme, then we pay attention only to the operator set $C(s)$, without bothering about its related subgroup chain. In such cases, the eigenvalue of $C(s)$ is used merely to distinguish between the components of an irreducible basis, and $C(s)$ can be chosen differently for different irreps. The choice of $C(s)$ can be arbitrary so long as its eigenvalues can provide enough labels for the basis vectors of the same irrep. It is always desirable that $C(s)$ contains as few operators as possible. For example, for two-dimensional irreps possible choices of $C(s)$ are a (plane) reflection operator σ, or a two-fold rotation C_2; for irreps with $h_\nu = 3(4)$ it is a three-fold (four-fold) rotation C_3 (C_4); and for irreps with $h_\nu = 6$, it is (C_{2x}, C_{2y}, I) or (C^+_{31}, I) where I is an inversion.

10.14.3. The irreps of $\mathbf{G}'_\mathbf{k}$ and the projective irreps of $\mathbf{G}_0(\mathbf{k})$

With the standard phase choice for the eigenvectors $P^{(\mathbf{k})(\nu)b}_a$, the irreducible matrix elements of $\mathbf{G}'_\mathbf{k}$ are simply related to the coefficients $u^{(\mathbf{k})(\nu)}_{ab,i}$ by [compare with Eq. (3-198)],

$$\begin{aligned} D^{(\mathbf{k})(\nu)}_{ab}(R_i) &= \Delta^{(\nu)}_{ab}(\gamma_i) \\ &= \sqrt{\frac{|\mathbf{G}_0(\mathbf{k})|}{h_\nu}}\,(u^{(\mathbf{k})(\nu)}_{ab,i})^* \ . \end{aligned} \tag{10-88}$$

By solving the eigenequation (3-176) we can obtain all the irreps $D^{(\mathbf{k})(\nu)}$ of $\mathbf{G}'_k$, or in other words obtain the projective irreps $\Delta^{(\nu)}$ of the little co-group $\mathbf{G}_0(\mathbf{k})$.

The rule for determining the phases of $P^{(\mathbf{k})(\nu)b}_a$ so that (10-88) holds is identical to that given in Sec. 3.9 under the substitution (10-87).

From (3-200) and (10-88) we get the two orthogonal theorems for the projective irreps of $\mathbf{G}_0(\mathbf{k})$,

$$\frac{h_\nu}{|\mathbf{G}_0(\mathbf{k})|} \sum_{i=1}^{|\mathbf{G}_0(\mathbf{k})|} \Delta^{(\nu)}_{ab}(\gamma_i)^* \Delta^{(\nu')}_{a'b'}(\gamma_i) = \delta_{\nu\nu'}\delta_{aa'}\delta_{bb'} \ , \tag{10-89a}$$

$$\sum_{\nu=1}^{n} \sum_{a,b=1}^{h_\nu} \frac{h_\nu}{|\mathbf{G}_0(\mathbf{k})|} \Delta^{(\nu)}_{ab}(\gamma_i)^* \Delta^{(\nu)}_{ab}(\gamma_j) = \delta_{ij} \ . \tag{10-89b}$$

Inserting (10-88) into (10-86), we get the normalized projection operator,

$$P^{(\mathbf{k})(\nu)b}_a = \sqrt{\frac{h_\nu}{|\mathbf{G}_0(\mathbf{k})|}} \sum_{i=1}^{|\mathbf{G}_0(\mathbf{k})|} D^{(k)(\nu)}_{ab}(R_i)^* R_i \tag{10-90}$$

for the rep group $\mathbf{G}'_\mathbf{k}$. The projection operator for the rep group $\mathbf{G}'_\mathbf{k}$ or for the little group $\mathbf{G}(\mathbf{k})$ is

$$P^{(\mathbf{k})(\nu)}_{ab} = \frac{h_\nu}{|\mathbf{G}_0(\mathbf{k})|} \sum_{i=1}^{|\mathbf{G}_0(\mathbf{k})|} D^{(\mathbf{k})(\nu)}_{ab}(R_i)^* R_i \ . \tag{10-91a}$$

Using Eqs. (10-66) and (10-71a) we can rewrite Eq. (10-91a) as

$$P_{ab}^{(\mathbf{k})(\nu)} = \frac{h_\nu}{|\mathbf{G}_0(\mathbf{k})|} \sum_{i=1}^{|\mathbf{G}_0(\mathbf{k})|} D_{ab}^{(\mathbf{k})(\nu)}(\{\gamma_i|\mathbf{V}(\gamma_i)\})^* \{\gamma_i|\mathbf{V}(\gamma_i)\} \ . \tag{10-91b}$$

10.14.4. The irreducible basis of $\mathbf{G}(\mathbf{k})$

The $\mathbf{G}'_\mathbf{k} \supset \mathbf{G}'_s$ and $\overline{\mathbf{G}}'_\mathbf{k} \supset \overline{\mathbf{G}}'_s$ irreducible basis in the rep space $\mathcal{L}(\mathbf{k})$ is given by

$$\psi_{\mathbf{k},a}^{(\nu)b} = P_a^{(\mathbf{k})(\nu)b} \psi_\mathbf{k}(\mathbf{x}) = \sum_{i=1}^{|\mathbf{G}_0(\mathbf{k})|} u_{ab,i}^{(\mathbf{k})(\nu)} \psi_i \ . \tag{10-92}$$

Notice that $\psi_{\mathbf{k},a}^{(\nu)b}$ is also the $\mathbf{G}(\mathbf{k}) \supset \mathbf{G}(s)$ and $\overline{\mathbf{G}}(\mathbf{k}) \supset \overline{\mathbf{G}}(s)$ irreducible basis, where $\mathbf{G}(s)$ is the subgroup of the little group $\mathbf{G}(\mathbf{k})$, which has $\mathbf{G}'_s$ of (10-81) as its rep group.

Under the action of the element $\{\gamma|\mathbf{c}\}$ of $\mathbf{G}(\mathbf{k})$ $\left[\overline{\{\gamma|\mathbf{c}\}}\right.$ of $\left.\overline{\mathbf{G}}(\mathbf{k})\right], \psi_{\mathbf{k}a}^{(\nu)b}$ changes only its "external" (intrinsic) quantum number $a(b)$

$$\{\gamma|\mathbf{c}\}\psi_{\mathbf{k},a}^{(\nu)b} = \sum_{a'} D_{a'a}^{(\mathbf{k})(\nu)}(\{\gamma|\mathbf{c}\})\psi_{\mathbf{k},a'}^{(\nu)b} \ , \tag{10-93a}$$

$$\overline{\{\gamma|\mathbf{c}\}}\psi_{\mathbf{k},a}^{(\nu)b} = \sum_{b'} D_{bb'}^{(k)(\nu)}(\{\gamma|\mathbf{c}\})\psi_{\mathbf{k},a}^{(\nu)b'} \ . \tag{10-93b}$$

The h_ν sets of irreducible bases of $\mathbf{G}(\mathbf{k})$, $\{\psi_{\mathbf{k},a}^{(\nu)b} : a = 1, 2, \ldots, h_\nu\}, b = 1, 2, \ldots, h_\nu$, which carry h_ν equivalent (or identical under the standard phase choice) irreps of $\mathbf{G}(\mathbf{k})$, are distinguished by the intrinsic quantum number b.

10.15. Example: The Point W of O_h^7

In this section, we give several examples of the application of the EFM for obtaining the characters and irreps of the rep group $\mathbf{G}'_\mathbf{k}$. From these it is then trivial to use (10-71b) to obtain the characters and small reps of the little group $\mathbf{G}(\mathbf{k})$.

Since cases (1)–(3) in Sec. 10.13 are trivial, we treat only case (4) here, the case when $\mathbf{k}$ is a surface point and the little group $\mathbf{G}(\mathbf{k})$ is non-symmorphic.

10.15.1. Seeking the CSCO and the characters of the point W of the space group O_h^7

The vector $\mathbf{p}$ for the point W is

$$\mathbf{p} = \left(\tfrac{1}{2}, \tfrac{1}{4}, \tfrac{3}{4}\right) \ . \tag{10-94}$$

O_h^7 belongs to the face-centered cubic Γ_c^f with the generators

$$\begin{aligned} &\{C_{2z}|0\} \ , \quad \{C_{2x}|0\} \ , \quad \{C_{31}^+|0\} \ , \\ &\{C_{2a}|\boldsymbol{\tau}\} \ , \quad \{I|\boldsymbol{\tau}\} \ , \quad \boldsymbol{\tau} = \left(\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}\right) \ . \end{aligned} \tag{10-95}$$

The little co-group is

$$\mathbf{G}_0(W) = D_{2d} = (\varepsilon, C_{2x}, C_{2d}, C_{2f}, \sigma_y, \sigma_z, S_{4x}^-, S_{4x}^+) \ , \quad |\mathbf{G}_0(W)| = 8 \ . \tag{10-96}$$

Using (10-80a) and Table 10.21-2 under the heading "cubic Γ_c^f" we can calculate the phase factor,

$$\eta_\rho = \exp[-2\pi i(\gamma_\rho \mathbf{p} - \mathbf{p}) \cdot \boldsymbol{\tau}] \ , \tag{10-97}$$

as shown in the first column of Table 10.15-1. $\eta_\rho = \pm 1, \pm i$. Hence the representation group $\mathbf{G}'_W$ is a four-fold covering group of D_{2d}.

Table 10.15-1. The group table of the rep group $\mathbf{G}'_W$ for the space group O_h^7.

η_ρ	$\{\epsilon\|0\}'$	$\{C_{2x}\|0\}'$	$\{C_{2d}\|\tau\}'$	$\{C_{2f}\|\tau\}'$	$\{\sigma_y\|\tau\}'$	$\{\sigma_z\|\tau\}'$	$\{S_{4z}^-\|0\}$	$\{S_{4z}^+\|0\}$
1	1	2	3	4	5	6	7	8
−1	2	1	−4	−3	−6	−5	8	7
i	3	4	$i1$	$i2$	$i7$	$i8$	5	6
$-i$	4	3	$-i2$	$-i1$	$-i8$	$-i7$	6	5
−1	5	6	−8	−7	−1	−2	4	5
1	6	5	7	7	2	1	3	4
i	7	8	$i6$	$i5$	$i3$	$i4$	2	1
$-i$	8	7	$-i5$	$-i6$	$-i4$	$-i3$	1	2

If we take up the group table of D_{2d}, and multiply the $(\rho\sigma)$ entries by the phase factor η_ρ for those columns σ which have the non-primitive translation τ, then we get the group table of the representation group $\mathbf{G}'_W$, shown in Table 10.15-1.

By multiplying the j-th column of Table 10.15-1 from the left with the element R_j^{-1} we obtain the class structure of $\mathbf{G}'_W$ shown in Table 10.15-2.

Table 10.15-2. The class structure of $\mathbf{G}'_W$.

$R_j^{-1}R_iR_j$ \ R_j / R_i	1	2	3	4	5	6	7	8
1	1	1	1	1	1	1	1	1
2	2	2	−2	−2	−2	−2	2	2
3	3	−3	3	−3	$-i4$	$i4$	$-i4$	$i4$
4	4	−4	−4	4	$i3$	$-i3$	$-i3$	$i3$
5	5	−5	$i6$	$-i6$	5	−5	$-i6$	$i6$
6	6	−6	$-i5$	$i5$	−6	6	$-i5$	$i5$
7	7	7	$i8$	$i8$	$i8$	$i8$	7	7
8	8	8	$-i7$	$-i7$	$-i7$	$-i7$	8	8

From Table 10.15-2 it is easily seen that $\mathbf{G}'_W$ has 14 classes with the class operators

$$
\begin{aligned}
&C_1 = R_1\ , \quad C_1' = iR_1\ , \quad C_1'' = -iR_1\ , \quad C_1''' = -R_1\ , \\
&C_2 = R_2 - R_2\ , \quad C_2' = iC_2\ , \quad C_3 = R_3 - R_3 + iR_4 - iR_4\ , \\
&C_3' = iC_3\ , \quad C_4 = R_5 - R_5 + iR_6 - iR_6\ , \quad C_4' = iC_4\ , \\
&C_5 = R_7 + iR_8\ , \quad C_5' = iC_5\ , \quad C_5'' = -iC_5\ , \quad C_5''' = -C_5\ .
\end{aligned}
\tag{10-98}
$$

However, only the class operators C_1 and C_5 are linearly independent. Hence $n = 2$. Using Table 10.15-1 we can easily establish the multiplication relation for the class operators C_1 and C_5,

$$
C_5 \begin{pmatrix} C_1 \\ C_5 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 2i & 0 \end{pmatrix} \begin{pmatrix} C_1 \\ C_5 \end{pmatrix} . \tag{10-99a}
$$

Then the representation matrix of C_5 in the class space is

$$
\mathcal{D}(C_5) = \begin{pmatrix} 0 & 2i \\ 1 & 0 \end{pmatrix} . \tag{10-99b}
$$

By diagonalizing $\mathcal{D}(C_5)$, we find that C_5 has two distinct eigenvalues $\nu = \pm(1+i)$; therefore C_5 is a CSCO–I of $\mathbf{G}'_W$. We could use the eigenvalues $\pm(1+i)$ to label the two irreps of $\mathbf{G}'_W$, but we prefer to use the conventional symbols W_1 and W_2 to label them.

The eigenvectors of $\mathcal{D}(C_5)$ with the normalization (3-43) (remembering that $g_1 = 1$ and $g_5 = 2$) are

$$\begin{aligned} &\nu = 1+i\ , \qquad \mathbf{q}^{(W_1)} = \tfrac{1}{\sqrt{8}}(2, 1-i)\ , \\ &\nu = -(1+i)\ , \quad \mathbf{q}^{(W_2)} = \tfrac{1}{\sqrt{8}}(2, -1+i)\ . \end{aligned} \tag{10-100}$$

From (3-245) and (10-100) we get the characters of the classes C_1 and C_5. Using (10-98) we in turn get the characters of the remaining classes. The complete character table is shown in Table 10.15-3.

Table 10.15-3. The character table of the rep group $\mathbf{G}'_W$ for the space group O_h^7.

		Class												
ν	(ν)	1	$1'$	$1''$	$1'''$	2	$2'$	3	$3'$	4	$4'$	5	$5'$	$5''$	$5'''$
$1+i$	W_1	2	$2i$	$-2i$	-2	0	0	0	0	0	0	$1+i$	$-1+i$	$1-i$	$-1-i$
$-(1+i)$	W_2	2	$2i$	$-2i$	-2	0	0	0	0	0	0	$-1-i$	$1-i$	$-1+i$	$1+i$

10.15.2. Obtaining the CSCO-I from the existing character table

For a group about which we know nothing except its group table, we can use the foregoing method to obtain the CSCO–I and characters of the group simultaneously. However, if the character table of a group is known, as is the case for all point groups and the 230 space groups, it is trivial to find the CSCO–I of the group by the method given in Sec. 3.12.

Now let us try to find the CSCO–I for the rep group $\mathbf{G}'_X$ of the space group O_h^7. The vector $\mathbf{p}$ for the point X is

$$\mathbf{p} = \left(\tfrac{1}{2}, \tfrac{1}{2}, 0\right)\ .$$

From Table T159 of Kovalev (1961), with slight changes in notation, we can write down the characters of the rep group $\mathbf{G}'_X$. We enter the characters of those elements whose characters are not identically zero in Table 10.15-4. Our X_i are related to Kovalev's $\hat{\tau}^i$ by; $X_1 \to \hat{\tau}^3$, $X_2 \to \hat{\tau}^4$, $X_3 \to \hat{\tau}^2$, $X_4 \to \hat{\tau}^1$.

Table 10.15-4. Character table of the rep group $\mathbf{G}'_X$ for the space group O_h^7.*

(C_1, C_2)	(ν)	$\{\varepsilon\|0\}'$	$\{C_{2x}\|0\}'$	$\{C_{2a}\|\tau\}'$	$\{C_{2b}\|\tau\}'$	$\{\sigma_{da}\|0\}'$	$\{\sigma_{db}\|0\}'$
(0,2)	X_1	2	2	0	0	2	2
(0, −2)	X_2	2	2	0	0	−2	−2
(2i, 0)	X_3	2	−2	2i	−2i	0	0
(−2i,0)	X_4	2	−2	−2i	2i	0	0

It is seen that $\{C_{2a}|\tau\}'$ and $-\{C_{2b}|\tau\}'$ belong to the same class, and $\{\sigma_{da}|0\}$ and $\{\sigma_{db}|0\}$ belong to the same class. Furthermore, according to (3-68), Table 10.15-4, after deleting the sixth and eighth columns, is (accidently) the eigenvalue table of the class operators. Hence we see that the class operators

$$\begin{aligned} C_1 &= \{C_{2a}|\tau\}' - \{C_{2b}|\tau\}'\ , \\ C_2 &= \{\sigma_{da}|0\} + \{\sigma_{db}|0\}\ , \end{aligned} \tag{10-101}$$

have $n = 4$ distinct sets of eigenvalues as shown in the first column of Table 10.15-4. Therefore, (C_1, C_2) is a CSCO–I of $\mathbf{G}'_X$.

10.15.3. Constructing irreps of the rep group $\mathbf{G}'_\mathbf{k}$. The Point W of O_h^7

With $n = 2$, and $|\mathbf{G}_0(W)| = 8$, (8-141b) becomes

$$8 = 2^2 + 2^2 \ . \tag{10-102}$$

Therefore, the eight–dimensional rep produced by the space $L(W)$ can be decomposed into two inequivalent irreps with dimension 2, each occurring twice. We choose

$$(C(s), \overline{C}(s)) = (R_7, \overline{R}_7) \ . \tag{10-103}$$

The matrices of the operators R_7 and $\overline{R}_7$ in the space $L(W)$ can be read out from the seventh row and seventh column, respectively, of Table 10.15-1. In the notation of (2-71),

$$\begin{aligned} D(R_7) &= \{7, 8, i6, i5, i3, i4, 2, 1\} \ , \\ D(\overline{R}_7) &= \{7, 8, 5, 6, 4, 3, 2, 1\} \ , \end{aligned} \tag{10-104}$$

These matrices are very much like the ordinary regular rep matrices, in that in each row and each column there is only one non–vanishing element.

The element $R_7 = \{S_{4x}^- | 0\}$ obeys the algebraic equation $(R_7)^4 = 1$. Hence the eigenvalues of R_7 are easily found to be $\pm 1, \pm i$. The same applies to the eigenvalues of $\overline{R}_7$.

Substituting the eigenvalues $a, b = \pm 1, \pm i$ into the eigenequations of $D(R_7)$ and $D(\overline{R}_7)$, we obtain eight simultaneous eigenvectors of $(R_7, \overline{R}_7)$ corresponding to the eight distinct sets of eigenvalues, $(a, b) = (1,1)(i,1), (1,i)(i,i), (-1,-1), (-i,-1)(-1,-i), (-i,-i)$. Therefore, $(R_7, \overline{R}_7)$ is already a CSCO–III of the group $\mathbf{G}'_W$, and the CSCO–I of $\mathbf{G}'_W$ is redundant in decomposing the rep space $L(\mathbf{k})$. Of course this happens only by accident. If we had chosen $(C(s), \overline{C}(s)) = (R_2, \overline{R}_2)$, the CSCO–III of $\mathbf{G}'_W$ would have had to include the CSCO–I of $\mathbf{G}'_W$. Hence a suitable choice of $C(s)$ can save a lot of work.

The eigenvectors are listed in Table 10.15-5.

From Eq. (10-85) we know that the first four vectors in Table 10.15-5 belong to an irrep labelled by W_1, and the other four vectors belong to another irrep labelled by W_2.

The phases of the eigenvectors in Table 10.15-5 are determined by the three steps given in Sec. 3.9.3. The phases for the first, fourth, fifth, and eighth rows are determined by step (1). The phases of the second and sixth rows can be chosen arbitrarily according to step (2). The phases of the third and seventh rows are determined by step (3). For example, from the first and second rows of Table 10.15-5 as well as from Table 10.15-1 we can evaluate

$$\begin{aligned} D_{12}^{(W_1)}(R_3) &= (\psi_1^{(W_1)1} | R_3 | \psi_i^{(W_1)1}\rangle \\ &= \tfrac{1}{4}\langle \mathbf{1+2+7+8} \,|\, \mathbf{3} \,|\, \mathbf{3+4+5+6}\rangle = i \ , \end{aligned}$$

where we used obvious abbreviations. Therefore, the coefficient in front of R_3 in the third row $\psi_1^{(W_1)b=2} \equiv \psi_1^{(W_1)i}$ must be proportional to $D_{12}^{(W_1)}(R_3)^* = -i$.

10.16. Irreducible Bases and Representations of the Space Group

10.16.1. The $\mathbf{k}$ *star*

We first factorize the space group $\mathbf{G}$ into left cosets with respect to the little group $\mathbf{G}(\mathbf{k})$,

$$\mathbf{G} = \mathbf{G}(\mathbf{k}) + \{\beta_2 | \mathbf{V}(\beta_2)\}\mathbf{G}(\mathbf{k}) + \ldots + \{\beta_q | \mathbf{V}(\beta_q)\}\mathbf{G}(\mathbf{k}) \ . \tag{10-105}$$

Table 10.15-5. Irreducible bases and irreps of the rep group $\mathbf{G}'_W$ for the space group O_h^7

$\psi_a^{(\nu)b}$	N		$\{\varepsilon\|0\}'$ R_1	$\{C_{2x}\|0\}'$ R_2	$\{C_{2d}\|0\}'$ R_3	$\{C_{2f}\|\tau\}'$ R_4	$\{\sigma_y\|\tau\}'$ R_5	$\{\sigma_z\|\tau\}'$ R_6	$\{S_{4x}^-\|0\}'$ R_7	$\{S_{4x}^+\|0\}'$ R_8
$\psi_1^{(W_1)1}$	$\frac{1}{2}$	D_{11}^*	1	1					1	1
$\psi_i^{(W_1)1}$	$\frac{1}{2}$	D_{21}^*			1	1	1	1		
$\psi_1^{(W_1)1}$	$\frac{1}{2}$	D_{12}^*			$-i$	i	-1	1		
$\psi_i^{(W_1)i}$	$\frac{1}{2}$	D_{22}^*	1	-1					$-i$	i
$\psi_{-1}^{(W_2)-1}$	$\frac{1}{2}$	D_{11}^*	1	1					-1	-1
$\psi_{-i}^{(W_2)-1}$	$\frac{1}{2}$	D_{21}^*			1	1	-1	-1		
$\psi_{-1}^{(W_2)-i}$	$\frac{1}{2}$	D_{12}^*			$-i$	i	1	-1		
$\psi_{-i}^{(W_2)-i}$	$\frac{1}{2}$	D_{22}^*	1	-1					i	$-i$
$\Delta^{(W_1)}(\gamma_i) = D^{(W_1)}(R_i)$			$\begin{bmatrix}1&0\\0&1\end{bmatrix}$	$\begin{bmatrix}1&0\\0&-1\end{bmatrix}$	$\begin{bmatrix}0&i\\1&0\end{bmatrix}$	$\begin{bmatrix}0&-i\\1&0\end{bmatrix}$	$\begin{bmatrix}0&-1\\1&0\end{bmatrix}$	$\begin{bmatrix}0&1\\1&0\end{bmatrix}$	$\begin{bmatrix}1&0\\0&i\end{bmatrix}$	$\begin{bmatrix}1&0\\0&-i\end{bmatrix}$
$\Delta^{(W_2)}(\gamma_i) = D^{(W_2)}(R_i)$			$\begin{bmatrix}1&0\\0&1\end{bmatrix}$	$\begin{bmatrix}1&0\\0&-1\end{bmatrix}$	$\begin{bmatrix}0&i\\1&0\end{bmatrix}$	$\begin{bmatrix}0&-i\\1&0\end{bmatrix}$	$\begin{bmatrix}0&1\\-1&0\end{bmatrix}$	$\begin{bmatrix}0&-1\\-1&0\end{bmatrix}$	$\begin{bmatrix}-1&0\\0&-i\end{bmatrix}$	$\begin{bmatrix}-1&0\\0&i\end{bmatrix}$

Suppose that $\psi_{\mathbf{k},a}^{(\nu)}$ is an irreducible basis of the little group $\mathbf{G}(\mathbf{k})$ and let us define

$$\psi_{\mathbf{k}_\sigma a}^{(\nu)} = \{\beta_\sigma|\mathbf{V}(\beta_\sigma)\}\psi_{\mathbf{k},a}^{(\nu)}\,, \quad \sigma = 1,2,\ldots,q; a = 1,2,\ldots,h_\nu\,, \tag{10-106}$$

with the convention that $\{\beta_1|\mathbf{V}(\beta_1)\} = \{\varepsilon|0\}$. The q wave vectors

$$\mathbf{k}_\sigma = \beta_\sigma \mathbf{k}\,, \quad \sigma = 1,2,\ldots,q \tag{10-107a}$$

form what is called a star, or set of mutually inequivalent $\mathbf{k}$ vectors

$$*\mathbf{k} = (\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_q)\,, \tag{10-107b}$$

with $\mathbf{k}_1 \equiv \mathbf{k}$. The wave vector $\mathbf{k}$ is called the canonical wave vector (Birman 1974). Any one of the q wave vectors can serve as the canonical wave vector. If $\mathbf{k}$ is a general point in the Brillouin zone, the $\mathbf{k}$ is called a general star, otherwise it is called a special star.

As an illustration, we consider the simple cubic lattice. The primitive translations are $\mathbf{t}_1 = a\mathbf{i}, \mathbf{t}_2 = a\mathbf{j}$, and $\mathbf{t}_3 = a\mathbf{k}$, while the basis vectors of the reciprocal lattice are $\mathbf{b}_1 = (2\pi/a)\mathbf{i}, \mathbf{b}_2 = (2\pi/a)\mathbf{j}, \mathbf{b}_3 = (2\pi/a)\mathbf{k}$. The Brillouin zone is shown in Fig. 10.16-1, which is the cubic bounded by the planes bisecting normally the vectors $\mathbf{b}_1, \mathbf{b}_2$ and $\mathbf{b}_3$. The special points are labelled by Γ, X, M, R (points of symmetry), and $\Delta, \Sigma, \Lambda, S, Z, T$ (lines or planes of symmetry). Let us find the symmetry group $\mathbf{G}_0(\mathbf{k})$ for each special point.

1. The star Γ. This is the point $\mathbf{k} = 0$. Its symmetry group is $\mathbf{G}_0(\mathbf{k}) = O_h$, with $|\mathbf{G}_0(\mathbf{k})| = |\mathbf{G}_0|$. The star consists of only one point. The little group is the space group itself, $\mathbf{G}(\mathbf{k}) = \mathbf{G}$.

2. Z. This is a general point on the intersection line of a face of the cube and the plane $k_z = 0$. It is sent into itself or an equivalent point under the group $C_{2v} = (e, \sigma_y, \sigma_z, C_{2x})$. Therefore,

$\mathbf{G}_0(\mathbf{k}) = \mathcal{C}_{2v}$ and is of order 4. The star consists of $q = 12$ points as shown in Fig. 10.16-2, where the four solid arms represent four points in the x–y plane (the other eight points are in the x–z and y–z planes), while the dashed arms represent the points equivalent to those represented by the solid arms.

3. Σ. The point is along the bisector of the angle between the axes $\mathbf{k}_x$ and $\mathbf{k}_y$ (see Fig. 10.16-3). The group $\mathbf{G}_0(\mathbf{k}) = \mathcal{C}_{2v}, \mathcal{C}_{2v} = (e, \sigma_b, \sigma_z, C_{2a})$. $|\mathbf{G}_0(\mathbf{k})| = 4$ and $q = 12$.

4. Δ. This point is on the k_y axis. $\mathbf{G}_0(\mathbf{k}) = \mathcal{C}_{4v}$ with k_y as the four-fold axis. $|\mathbf{G}_0(\mathbf{k})| = 8$ and $q = 6$. The star contains six points, four points in the x–y plane (see Fig. 10.16-4) and the other two in the directions of $\mathbf{k}_z$ and $-\mathbf{k}_z$ respectively.

5. X. X is the intersection of the $\mathbf{k}_y$ axis with a face of the cube. $\mathbf{G}_0(\mathbf{k}) = D_{4h}$ (with $\mathbf{k}_y$ as the four-fold axis). $|\mathbf{G}_0(\mathbf{k})| = 16$ and $q = 3$. The star contains three points X, X' and X'', as shown in Fig. 10.16-1 and Fig. 10.16-5.

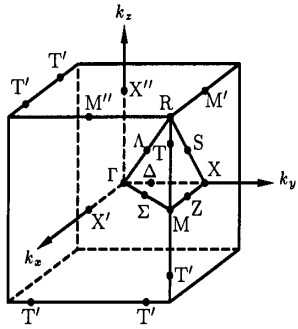


Fig. 10.16-1. The Brillouin zone for simple cubic.

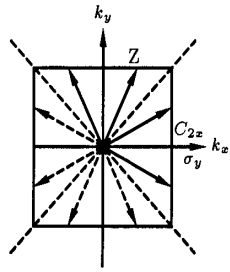


Fig. 10.16-2. The star Z; $q = 12$, $\mathbf{G}_0(\mathbf{k}) = \mathcal{C}_{2v}$ $(e, \sigma_y, \sigma_z, C_{2x})$.

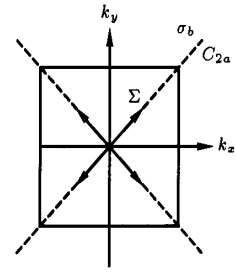


Fig. 10.16-3. The star Σ: $q = 12$, $\mathbf{G}_0(\mathbf{k}) = (e, \sigma_b, \sigma_z, C_{2a})$.

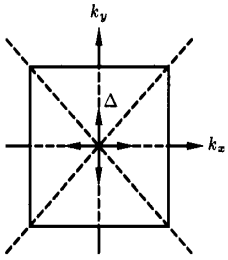


Fig. 10.16-4. The star Δ: $q = 6$, $\mathbf{G}_0(\mathbf{k}) = \mathcal{C}_{4v}$ (with $\mathbf{k}_y$ as the four-fold axis).

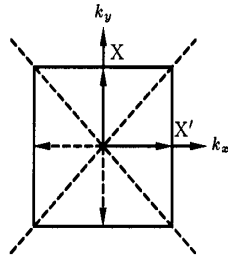


Fig. 10.16-5. The star X: $q = 3$, $\mathbf{G}_0\ (\mathbf{k}) = D_{4h}$ (with $\mathbf{k}_y$ as the four-fold axis).

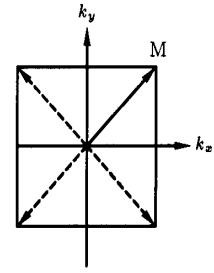


Fig. 10.16-6. The star M: $q = 3$, $\mathbf{G}_0\ (\mathbf{k}) = D_{4h}$ (with $\mathbf{k}_z$ as the four-fold axis).

6. M. $\mathbf{G}_0(\mathbf{k}) = D_{4h}$ (with $\mathbf{k}_z$ as the four-fold axis as in Fig. 10.16-6). $|\mathbf{G}_0(\mathbf{k})| = 16$ and $q = 3$. The star contains three points M, M', and M'' (Fig. 10.16-1).

7. T. $\mathbf{G}_0(\mathbf{k}) = \mathcal{C}_{4v}$ (with $\mathbf{k}_z$ as the four-fold axis). $|\mathbf{G}_0(\mathbf{k})| = 8$ and $q = 6$. The star consists of six points (Fig. 10.16-1).

8. Λ. $\mathbf{G}_0(\mathbf{k}) = \mathcal{C}_{3v}$ (with the line $\Gamma\Delta$ as the three-fold axis). $|\mathbf{G}_0(\mathbf{k})| = 6$ and $q = 8$.

9. R. $\mathbf{G}_0(\mathbf{k}) = \mathbf{G}_0 = O_h$. The star consists of only one point.

10.16.2. The induced representation

The space

$$\mathcal{L}(\mathbf{k}_\sigma) = \{\psi^{(\nu)}_{\mathbf{k}_\sigma a}: \quad a = 1, 2, \ldots, h_\nu\} \tag{10-108a}$$

is isomorphic to the space $\mathcal{L}(\mathbf{k})$, or to the group space $L(\mathbf{k})$ of the rep group $\mathbf{G}'_\mathbf{k}$. Clearly, the space $\mathcal{L}(*k)$ defined by (10-55c) is decomposed into a direct sum of the q spaces $\mathcal{L}(\mathbf{k}_\sigma)$ isomorphic to one another,

$$\mathcal{L}(*\mathbf{k}) = \sum_{\sigma=1}^{q} \oplus \mathcal{L}(\mathbf{k}_\sigma) \; . \tag{10-108b}$$

Let us apply an element $\{\alpha|\mathbf{a}\}$ of $\mathbf{G}$ to (10-106),

$$\{\alpha|\mathbf{a}\}\psi^{(\nu)}_{\mathbf{k}_\sigma a} = \{\alpha|\mathbf{a}\}\{\beta_\sigma|\mathbf{v}_\sigma\}\psi^{(\nu)}_{\mathbf{k},a} \; . \tag{10-109}$$

$\{\alpha|\mathbf{a}\}\{\beta_\sigma|V_\sigma\}$ must be an element of $\mathbf{G}$ and must belong to one and only one coset, say the τ–th coset, that is,

$$\{\alpha|\mathbf{a}\}\{\beta_\sigma|\mathbf{V}_\sigma\} = \{\beta_\tau|\mathbf{V}_\tau\}\{\gamma|\mathbf{c}\} \; . \tag{10-110}$$

Assembling (10-106), (10-110) and (10-93a), we obtain

$$\begin{aligned}\{\alpha|\mathbf{a}\}\psi^{(\nu)}_{\mathbf{k}_\sigma a} &= \{\beta_\tau|\mathbf{V}_\tau\}\sum_b D^{(\mathbf{k})(\nu)}_{ba}(\{\gamma|\mathbf{c}\})\psi^{(\nu)}_{\mathbf{k},b} \\ &= \sum_b D^{(\mathbf{k})(\nu)}_{ba}(\{\gamma|\mathbf{c}\})\psi^{(\nu)}_{\mathbf{k}_\tau,b} \; ,\end{aligned} \tag{10-111}$$

where $D^{(\mathbf{k})(\nu)}(\{\gamma|\mathbf{c}\})$ is the irreducible matrix of the little group $\mathbf{G}(\mathbf{k})$. Therefore, the qh_ν functions $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ carry a rep for the space group $\mathbf{G}$, which is the induced rep (Sec. 2.10) and denoted by $D^{(*\mathbf{k})(\nu)}$ (Birman 1974) or $D^{(\mathbf{k})(\nu)} \uparrow \mathbf{G}$ (Bradley 1972). It can be proved that the induced rep $D^{(*\mathbf{k})(\nu)}$ is an irrep of the space group $\mathbf{G}$ (Chen, Gao & Ma 1985).

The induced rep is of dimension qh_ν, and its matrix elements can be expressed as

$$D^{(*\mathbf{k}),(\nu)}_{\tau b,\sigma a}(\{\alpha|\mathbf{a}\}) = \langle\psi^{(\nu)}_{\mathbf{k}_\tau b}|\{\alpha|\mathbf{a}\}|\psi^{(\nu)}_{\mathbf{k}_\sigma a}\rangle \; . \tag{10-112a}$$

Define

$$R_{\bar{\tau}\alpha\sigma} \equiv \{\beta_\tau|\mathbf{V}_\tau\}^{-1}\{\alpha|\mathbf{a}\}\{\beta_\sigma|\mathbf{V}_\sigma\} \; . \tag{10-112b}$$

It follows from (10-106) and (10-112a) that

$$D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}(\{\alpha|\mathbf{a}\}) = \langle\psi^{(\nu)}_{\mathbf{k},b}|R_{\bar{\tau}\alpha\sigma}|\psi^{(\nu)}_{\mathbf{k},a}\rangle \; . \tag{10-112c}$$

According to the left coset decomposition (10-105), we know that $R_{\bar{\tau}\alpha\sigma}$ is either an element of the little group $\mathbf{G}(\mathbf{k})$ or a coset representative $\{\beta|\mathbf{V}(\beta)\}$ times an element of $\mathbf{G}(\mathbf{k})$. For the former, the right–hand side of (10-112c) is just the irreducible matrix element of $\mathbf{G}(\mathbf{k})$. For the latter, (10-112c) must vanish since $R_{\bar{\tau}\alpha\sigma} = \{\beta|\mathbf{V}(\beta)\}\{\gamma|\mathbf{c}\}$ will change the wave vector $\mathbf{k}$ into $\mathbf{k}_\beta$, while $\mathbf{k}$ is the label for the irreps of the translational group $\mathbf{T}$ and the bases belonging to different irreps of $\mathbf{T}$ are orthogonal. Hence (10-112c) can be expressed as [compare with (2-106h)]

$$\begin{aligned}D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}(\{\alpha|\mathbf{a}\}) &= D^{(\mathbf{k})(\nu)}_{ba}(R_{\bar{\tau}\alpha\sigma}) \\ &= D^{(\mathbf{k})(\nu)}_{ba}(\{\beta_\tau|\mathbf{V}_\tau\}^{-1}\{\alpha|\mathbf{a}\}\{\beta_\sigma|\mathbf{V}_\sigma\}) \; .\end{aligned} \tag{10-112d}$$

It is convenient to write the $qh_\nu \times qh_\nu$ matrix $D^{(*\mathbf{k})(\nu)}$ in block decomposition form (Birman 1974),

$$D^{(*\mathbf{k})(\nu)}(\{\alpha|\mathbf{a}\}) = \begin{pmatrix} D^{(*\mathbf{k})(\nu)}_{(11)} & \cdots & D^{(*\mathbf{k})(\nu)}_{(1q)} \\ \vdots & & \vdots \\ D^{(*\mathbf{k})(\nu)}_{(q1)} & \cdots & D^{(*\mathbf{k})(\nu)}_{(qq)} \end{pmatrix} , \tag{10-113a}$$

where

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\alpha|\mathbf{a}\}) = D^{(\mathbf{k})(\nu)}(\{\beta_\tau|\mathbf{V}_\tau\}^{-1}\{\alpha|\mathbf{a}\}\{\beta_\sigma|\mathbf{V}_\sigma\}) \tag{10-113b}$$

is a $(h_\nu \times h_\nu)$ matrix. According to (10-110), for given $\{\alpha|\mathbf{a}\}$ and σ there is only a unique τ that enables $R_{\overline{\tau}\alpha\sigma}$ to belong to the little group $\mathbf{G}(\mathbf{k})$. As a consequence, in each row and each column of the block form (10-113a), only one matrix block differs from zero. Another way of saying this is that for given σ and τ, only those elements of $\mathbf{G}$ which satisfy

$$\{\alpha|\mathbf{V}(\alpha)+\mathbf{R}_n\} = \{\beta_\tau|\mathbf{V}_\tau\}\{\gamma|\mathbf{V}(\gamma)+\mathbf{R}_m\}\{\beta_\sigma|\mathbf{V}_\sigma\}^{-1} , \quad \gamma \in \mathbf{G}_0(\mathbf{k}) \tag{10-113c}$$

have the non–zero submatrices

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\alpha|\mathbf{V}(\alpha)+\mathbf{R}_n\}) = D^{(\mathbf{k})(\nu)}(\{\gamma|\mathbf{V}(\gamma)+\mathbf{R}_m\}) \tag{10-113d}$$

Notice that there is a one–to–one correspondence between α and γ on the one hand, and $\mathbf{R}_n$ and $\mathbf{R}_m$ on the other hand.

10.16.3. A simple algorithm for full rep matrices

To go further, we note that although (10-113d) is simple in appearance, it is not the best form for practical construction of the full matrices of a space group. In the following, we rewrite it in a more appropriate form.

From (10-113b) and (10-9) we have

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\alpha|\mathbf{a}\}) = D^{(\mathbf{k})(\nu)}(\{\beta_\tau^{-1}\alpha\beta_\sigma|\beta_\tau^{-1}(\alpha\mathbf{V}_\sigma - \mathbf{V}_\tau + \mathbf{a})\}) . \tag{10-113e}$$

With the help of (10-71c) and $\exp[-i\mathbf{k}\cdot\beta_\tau^{-1}(\alpha\mathbf{V}_\sigma)] = \exp[-i\mathbf{k}_\tau\cdot(\alpha\mathbf{V}_\sigma)]$, this becomes

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\alpha|\mathbf{a}\}) = \exp[-i\mathbf{k}_\tau\cdot(\alpha\mathbf{V}_\sigma - \mathbf{V}_\tau + \mathbf{a})]\mathcal{D}_{(\tau\sigma)}(\alpha) , \tag{10-114a}$$

where

$$\mathcal{D}_{(\tau\sigma)}(\alpha) \equiv \Delta(\beta_\tau^{-1}\alpha\beta_\sigma) , \tag{10-114b}$$

with the convention

$$\Delta(\beta_\tau^{-1}\alpha\beta_\sigma) = 0 \quad \text{if} \quad \beta_\tau^{-1}\alpha\beta_\sigma \notin \mathbf{G}_0(\mathbf{k}) . \tag{10-114c}$$

In other words,

$$\Delta(\beta_\tau^{-1}\alpha\beta_\sigma) = 0 \tag{10-115a}$$

unless

$$\beta_\tau^{-1}\alpha\beta_\sigma = \gamma , \tag{10-115b}$$

or

$$\alpha\beta_\sigma = \beta_\tau\gamma . \tag{10-115c}$$

Multiplying (10-115c) from the right by $\mathbf{k}$, and using (10-107a), we obtain another form of condition (10-115b)

$$\alpha\mathbf{k}_\sigma \doteq \mathbf{k}_\tau . \tag{10-115d}$$

Setting $\{\alpha|\mathbf{a}\} = \{\varepsilon|\mathbf{R}_n\}$, from (10-115d) we must have $\sigma = \tau$, while from (10-114) we have

$$\begin{aligned} D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\varepsilon|\mathbf{R}_n\}) &= \delta_{\tau\sigma}\exp(-i\mathbf{k}_\tau \cdot \mathbf{R}_n)\Delta(\varepsilon) \\ &= \delta_{\tau\sigma}\exp(-i\mathbf{k}_\tau \cdot \mathbf{R}_n)\mathbf{I}_\nu \ , \end{aligned} \tag{10-116}$$

where $\mathbf{I}_\nu$ is the $h_\nu \times h_\nu$ unit matrix.

Hence we see that the translation $\{\varepsilon|\mathbf{R}_n\}$ is represented by the diagonal matrix

$$D^{(*\mathbf{k})(\nu)}(\{\varepsilon|\mathbf{R}_n\}) = \begin{pmatrix} e^{-i\mathbf{k}_1 \cdot \mathbf{R}_n}\mathbf{I}_\nu & & \\ & \ddots & \\ & & e^{-i\mathbf{k}_q \cdot \mathbf{R}_n}\mathbf{I}_\nu \end{pmatrix} . \tag{10-117}$$

Equation (10-114) gives a very convenient formula for constructing irreps of the space group $\mathbf{G}$ from the irreps $\Delta(\gamma) = D^{(\mathbf{k})(\nu)}(\{\gamma|\mathbf{V}(\gamma)\}')$ of the rep group $\mathbf{G}'_\mathbf{k}$. The procedure for obtaining irreps of $\mathbf{G}$ can be summarized as follows.

1. Following our procedure for (10-113a), we first introduce a matrix $\mathcal{D}(\{\alpha|\mathbf{a}\})$, whose $(\sigma\tau)$ block is the matrix $\mathcal{D}_{(\tau\sigma)}(\{\alpha|\mathbf{a}\})$ defined by (10-114b). To obtain $\mathcal{D}(\{\alpha|\mathbf{a}\})$, let us build up an array with q rows labelled by $\varepsilon, \beta_2^{-1}, \ldots, \beta_q^{-1}$ and q columns labelled by $\varepsilon, \beta_2, \ldots, \beta_q$,

$$\mathcal{D}(\{\alpha|\mathbf{a}\}) = \begin{array}{c} \\ \varepsilon \\ \beta_2^{-1} \\ \vdots \\ \beta_\tau^{-1} \\ \vdots \\ \beta_q^{-1} \end{array} \begin{array}{c} \begin{array}{cccccc} \varepsilon & \beta_2 & \ldots & \beta_\sigma & \ldots & \beta_q \end{array} \\ \begin{pmatrix} & & & 0 & & \\ & & & 0 & & \\ & & & \vdots & & \\ 0 & 0 & \ldots & \Delta(\gamma) & \ldots & 0 \\ & & & \vdots & & \\ & & & 0 & & \end{pmatrix} \end{array} \quad \text{for} \quad \beta_\tau^{-1}\alpha\beta_\sigma = \gamma \ . \tag{10-118}$$

Utilizing the point group multiplication table, we form the products $\beta_\tau^{-1}\alpha\beta_\sigma$ for given τ with varying $\sigma = 1, 2, \ldots$. In each step we check whether $\beta_\tau^{-1}\alpha\beta_\sigma$ is an element of the point group $\mathbf{G}_0(\mathbf{k})$. If not, we put a zero (an $h_\nu \times h_\nu$ null matrix) in the $(\tau\sigma)$ block; if it is an element, for example $\beta_\tau^{-1}\alpha\beta_\sigma = \gamma$, then we put $\Delta(\gamma)$ into the $(\tau\sigma)$ block and zero for all the remaining entries in the τ-th row and σ-th column. We repeat this process for each $\tau = 1, 2, \ldots, q$.

2. Multiplying the nonzero matrices $\Delta(\gamma)$ in Eq. (10-118) by the appropriate phase factors $\exp[-i\mathbf{k}_\tau \cdot (\alpha\mathbf{V}_\sigma - \mathbf{V}_\tau + \mathbf{a})]$, we immediately get the sought-for matrix $D^{(*\mathbf{k})(\nu)}(\{\alpha|\mathbf{a}\})$.

3. The following symmetries (10-119) of the matrix $\mathcal{D}(\{\alpha|\mathbf{a}\})$ can be used either to save work or to check the calculation.

From (10-114b) it is seen that if

$$\mathcal{D}_{(\tau\sigma)}(\{\alpha|\mathbf{a}\}) = \Delta(\gamma) \ , \quad \gamma = \beta_\tau^{-1}\alpha\beta_\sigma \ , \tag{10-119a}$$

then

$$\mathcal{D}_{(\sigma\tau)}(\{\alpha|\mathbf{a}\}^{-1}) = \Delta(\gamma^{-1}) \ . \tag{10-119b}$$

Furthermore, if $\alpha = \alpha^{-1}$, we have

$$\mathcal{D}_{(\sigma\tau)}(\{\alpha|\mathbf{a}\}) = \Delta(\gamma^{-1}) \ , \tag{10-119c}$$

since

$$\mathcal{D}_{(\sigma\tau)}(\{\alpha|\mathbf{a}\}) = \Delta(\beta_\sigma^{-1}\alpha\beta_\tau) = \Delta((\beta_\tau^{-1}\alpha\beta_\sigma)^{-1}) \ .$$

For examples of these symmetries, see (10-175) and (10-186).

From the foregoing discussion we see that in the process of constructing irreps of the space group we are able to avoid tedious space group multiplication, and only the much simpler point-group multiplication is required.

Another point that deserves mention is that the choice of the coset representative $\{\beta_\sigma|\mathbf{V}_\sigma\}$ is arbitrary, that is, any element in a coset can be chosen as the representative of that coset. Different choices of the representatives correspond to different conventions for relative phases between the basis vectors $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ with different σ. For practical purposes, it is always desirable to choose elements not associated with non-primitive translations as the coset representatives, since under such a choice (10-114) simplifies to follows:

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\alpha|\mathbf{a}\}) = \exp(-i\mathbf{k}_\tau \cdot \mathbf{a})\Delta(\beta_\tau^{-1}\alpha\beta_\sigma) \ , \tag{10-120}$$

which is suitable only when $\mathbf{V}(\beta_\sigma) = \mathbf{V}(\beta_\tau) = 0$.

10.16.4. The $\mathbf{G} \supset \mathbf{G}(\mathbf{k}_\sigma) \supset \mathbf{G}(s_\sigma) \supset \mathbf{T}$ *irreducible basis*

Finally let us take a look at the meaning of the irreducible basis vectors $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ of the space group $\mathbf{G}$. We have already seen that $\psi^{(\nu)}_{\mathbf{k},a}$ is the $\mathbf{G} \supset \mathbf{G}(\mathbf{k}) \supset \mathbf{G}(s) \supset \mathbf{T}$ irreducible basis and obeys the eigenequations

$$\begin{pmatrix} C \\ C(s) \\ \widehat{\mathbf{k}} \end{pmatrix} \psi^{(\nu)}_{\mathbf{k},a} = \begin{pmatrix} \nu \\ a \\ \mathbf{k} \end{pmatrix} \psi^{(\nu)}_{\mathbf{k},a} \ , \tag{10-121}$$

where C and $C(s)$ are the CSCO-I of the rep groups $\mathbf{G}'_\mathbf{k}$ and $\mathbf{G}'_s$ respectively, and $\widehat{\mathbf{k}} = -i\nabla$ is the CSCO-I of $\mathbf{T}$. The little group $\mathbf{G}(\mathbf{k})$ and the rep group $\mathbf{G}'_\mathbf{k}$ have common irreducible bases and common irrep labels. For convenience, we shall refer to the CSCO-I C of $\mathbf{G}'_\mathbf{k}$ as the CSCO-I of the little group $\mathbf{G}(\mathbf{k})$; similarly, the CSCO-I $C(s)$ of $\mathbf{G}'_s$ will be referred to as the CSCO-I of the subgroup $\mathbf{G}(s)$ of $\mathbf{G}(\mathbf{k})$.

As in (10-56) we may define the little group $\mathbf{G}(\mathbf{k}_\sigma)$ for the wave vector $\mathbf{k}_\sigma = \beta_\sigma\mathbf{k}$ such that under the operations of the rotational part of $\mathbf{G}(\mathbf{k}_\sigma)$, the wave vector $\mathbf{k}_\sigma$ is invariant modulo a reciprocal lattice vector. Clearly the relation between the groups $\mathbf{G}(\mathbf{k}_\sigma)$ and $\mathbf{G}(\mathbf{k})$ is

$$\mathbf{G}(\mathbf{k}_\sigma) = \{\beta_\sigma|\mathbf{V}_\sigma\}\mathbf{G}(\mathbf{k})\{\beta_\sigma|\mathbf{V}_\sigma\}^{-1} \ . \tag{10-122a}$$

Suppose $\{\alpha|\mathbf{a}\}$ is an element of $\mathbf{G}(\mathbf{k}_\sigma)$; then $\{\alpha|\mathbf{a}\}$ is necessarily of the form

$$\{\alpha|\mathbf{a}\} = \{\beta_\sigma|\mathbf{V}_\sigma\}\{\gamma|\mathbf{V}(\gamma) + \mathbf{R}_n\}\{\beta_\sigma|\mathbf{V}_\sigma\}^{-1} \ . \tag{10-123a}$$

From (10-123a) and (10-111) we have

$$\{\alpha|\mathbf{a}\}\psi^{(\nu)}_{\mathbf{k}_\sigma a} = \sum_b D^{(\mathbf{k})(\nu)}_{ba}(\{\gamma|\mathbf{V}(\gamma) + \mathbf{R}_n\})\psi^{(\nu)}_{\mathbf{k}_\sigma b} \ , \tag{10-123b}$$

that is, $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ is the irreducible basis of the group $\mathbf{G}(\mathbf{k}_\sigma)$. Furthermore, as in (10-122a), we define

$$\mathbf{G}(s_\sigma) \equiv \{\beta_\sigma|\mathbf{V}_\sigma\}\mathbf{G}(s)\{\beta_\sigma|\mathbf{V}_\sigma\}^{-1} \ . \tag{10-122b}$$

Clearly $\mathbf{G}(s_\sigma)$ is a subgroup of $\mathbf{G}(\mathbf{k}_\sigma)$. According to Eq. (10-122), the CSCO-I of $\mathbf{G}(\mathbf{k}_\sigma)$ and $\mathbf{G}(s_\sigma)$ are

$$C(\mathbf{k}_\sigma) = \{\beta_\sigma|\mathbf{V}_\sigma\}C\{\beta_\sigma|\mathbf{V}_\sigma\}^{-1} \ ,$$

$$C(s_\sigma) = \{\beta_\sigma|\mathbf{V}_\sigma\}C(s)\{\beta_\sigma|\mathbf{V}_\sigma\}^{-1} \ . \tag{10-124}$$

With (10-106), (10-121) and (10-124) we have

$$\begin{pmatrix} C(\mathbf{k}_\sigma) \\ C(s_\sigma) \\ \widehat{\mathbf{k}} \end{pmatrix} \psi^{(\nu)}_{\mathbf{k}_\sigma a} = \begin{pmatrix} \nu \\ a \\ \mathbf{k}_\sigma \end{pmatrix} \psi^{(\nu)}_{\mathbf{k}_\sigma a} \,. \tag{10-125}$$

Hence we see that the partner (or component) $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ of the irreducible basis of a space group $\mathbf{G}$ is the $\mathbf{G} \supset \mathbf{G}(\mathbf{k}_\sigma) \supset \mathbf{G}(s_\sigma) \supset \mathbf{T}$ irreducible basis. In other words, the group chains used to classify the irreducible basis vectors of a space group $\mathbf{G}$ vary with the components. This is quite different from the usual case (for example the permutation group, rotation group, or unitary group), where the same group chain is always used to classify all the components in a given irrep of the group.

10.17. The Irreducible Basis and Matrices of C^4_{2v}

C^4_{2v} is a non-symmorphic space group, $\mathbf{G}_0 = C_{2v}$. It belongs to the simple orthorhombic lattice. The three perpendicular primitive translations are

$$\mathbf{t}_1 = a\mathbf{i} \,, \quad \mathbf{t}_2 = b\mathbf{j} \,, \quad t_3 = c\mathbf{k} \,.$$

The group elements are specified by

$$\mathcal{R}_1 = \{\varepsilon|0\} \,, \quad \mathcal{R}_2 = \{\sigma_x|\mathbf{v}\} \,, \quad \mathcal{R}_3 = \{\sigma_y|\mathbf{v}\} \,, \quad \mathcal{R}_4 = \{C_{2z}|0\} \,, \quad \mathbf{v} = \mathbf{t}_1/2 \,. \tag{10-126}$$

The arrangement of the atoms in the x–y plane is shown in Fig. 10.17-1. The basis vectors for the reciprocal lattice are

$$\mathbf{b}_1 = \frac{2\pi}{a}\mathbf{i}, \quad \mathbf{b}_2 = \frac{2\pi}{b}\mathbf{j}, \quad \mathbf{b}_3 = \frac{2\pi}{c}\mathbf{k} \,.$$

The Brillouin zone is shown in Fig. 10.17-2.

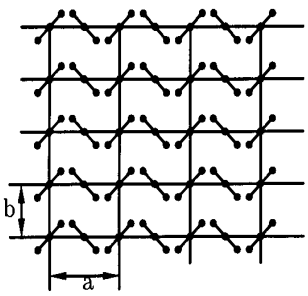


Fig. 10.17-1. The arrangement of the atoms in the xy plane for a crystal with C^4_{2v} symmetry

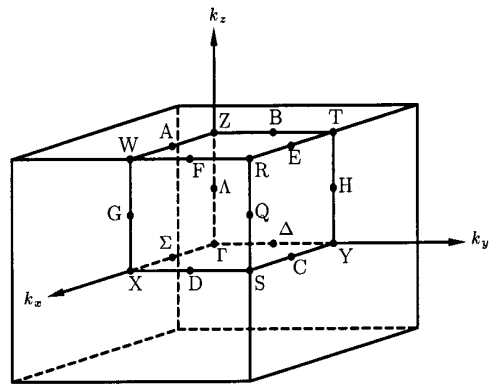


Fig. 10.17-2. The Brillouin zone for the simple orthorhombic lattice.

In the following we shall consider the irreducible bases and irreps for four stars.

10.17.1. A general star: $\mathbf{p} = (p_1, p_2, p_3)$.

$\mathbf{G}_0(\mathbf{k}) = \varepsilon, \mathbf{G}(k) = \mathbf{T}$. The irrep of the rep group is $\Delta(\varepsilon) = 1$. The irreducible basis of $\mathbf{G}(\mathbf{k})$ is

$$\psi_{\mathbf{k}} = \exp\left[i(\mathbf{k} + \mathbf{K}_m) \cdot \mathbf{r}\right] = \exp\left[2\pi i \sum_j \kappa_j \xi_j\right] \,, \quad \kappa_j = p_j + m_j \,. \tag{10-127}$$

The group elements in (10-126) are just the coset representatives $\{\beta_i|\mathbf{V}(\beta_i)\}$. The induced basis, that is, the irreducible basis of the space group, is

$$\begin{aligned}
\Psi_1 &= \mathcal{R}_1\psi_{\mathbf{k}} = \exp\left[2\pi i\sum_j \kappa_j\xi_j\right] , \\
\Psi_2 &= \mathcal{R}_2\psi_{\mathbf{k}} = \exp\left[i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{v}\right]\exp\left[2\pi i(-\kappa_1\xi_1+\kappa_2\xi_2+\kappa_3\xi_3)\right] , \\
\Psi_3 &= \mathcal{R}_3\psi_{\mathbf{k}} = \exp\left[-i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{v}\right]\exp\left[2\pi i(\kappa_1\xi_1-\kappa_2\xi_2+\kappa_3\xi_3)\right] , \\
\Psi_4 &= \mathcal{R}_4\psi_{\mathbf{k}} = \exp\left[2\pi i(-\kappa_1\xi_1-\kappa_2\xi_2+\kappa_3\xi_3)\right] .
\end{aligned} \tag{10-128}$$

The $\mathbf{k}$ star is

$$(*\mathbf{k}) = (p_1,p_2,p_3) , \quad (-p_1,p_2,p_3) , \quad (p_1,-p_2,p_3) , \quad (-p_1,-p_2,p_3) .$$

Using (10-118) we can find the matrices $\mathcal{D}(\{\alpha|\mathbf{a}\})$, for example,

$$\mathcal{D}(\{\sigma_x|\mathbf{v}\})=\left(\begin{array}{cc|cc} & \Delta(\varepsilon) & & \\ \Delta(\varepsilon) & & & \\ \hline & & & \Delta(\varepsilon) \\ & & \Delta(\varepsilon) & \end{array}\right) , \quad \mathcal{D}(\{\sigma_y|\mathbf{v}\})=\left(\begin{array}{cc|cc} & & & \Delta(\varepsilon) \\ & & & \Delta(\varepsilon) \\ \hline \Delta(\varepsilon) & & & \\ & \Delta(\varepsilon) & & \end{array}\right) . \tag{10-129}$$

From (10-114) and (10-129) we get the irreps of the space group C_{2v}^4,

$$D^{*(\mathbf{k})}(\{\varepsilon|\mathbf{R}_n\}) = \left(\begin{array}{cc|cc} e_1 & & & \\ & e_2 & & \\ \hline & & e_3 & \\ & & & e_4 \end{array}\right) , \quad D^{(*\mathbf{k})}(\{\sigma_x|\mathbf{v}\}) = \left(\begin{array}{cc|cc} 0 & 1 & & \\ 1 & 0 & & \\ \hline & & 0 & 1 \\ & & 1 & 0 \end{array}\right) , \tag{10-130}$$

$$D^{(*\mathbf{k})}(\{\sigma_y|\mathbf{v}\}) = \left(\begin{array}{cc|cc} & & e_1^2 & 0 \\ & & 0 & 1 \\ \hline 1 & 0 & & \\ 0 & (e_1^*)^2 & & \end{array}\right) , \quad D^{(*\mathbf{k})}(\{C_{2z}|0\}) = \left(\begin{array}{cc|cc} & & 0 & 1 \\ & & e_1^2 & 0 \\ \hline 0 & (e_1^*)^2 & & \\ 1 & 0 & & \end{array}\right) ,$$

where $e_j = \exp[-i\mathbf{k}_j\cdot\mathbf{R}_n]$.

10.17.2. The star $\Gamma : \mathbf{p} = (0,0,0)$.

$\mathbf{G}_0(\mathbf{k}) = \mathcal{C}_{2v}$ and the little group is the space group itself, $\mathbf{G}(\mathbf{k}) = \mathbf{G}$. The rep group $\mathbf{G}'_\Gamma$ is isomorphic to the point group $\mathcal{C}_{2v} = (\varepsilon,\sigma_x,\sigma_y,C_{2z})$. The irreps of $\mathcal{C}_{2v}$ are known and listed in Table 10.17-1.

Table 10.17-1. Irreps of $\mathcal{C}_{2v}$.

ν	e	σ_x	σ_y	C_{2z}
A_1	1	1	1	1
A_2	1	−1	−1	1
B_2	1	−1	1	−1
B_2	1	1	−1	−1

From (10-92) and Table 10.17-1 we get the irreducible basis of $\mathbf{G}(\mathbf{k}) = \mathbf{G}$,

$$\psi_{\mathbf{k}}^{(A_1)} = \tfrac{1}{2}(\psi_1 + \psi_2 + \psi_3 + \psi_4) = 2\begin{cases} \cos\mu_1\xi_1 \cos\mu_2\xi_2 \exp(i\mu_3\xi_3)\,, \\ \sin\mu_1\xi_1 \sin\mu_2\xi_2 \exp(i\mu_3\xi_3)\,, \end{cases} \quad \text{for} \quad m_1 = \begin{matrix}\text{even}\\ \text{odd,}\end{matrix}$$

$$\psi_{\mathbf{k}}^{(A_2)} = \tfrac{1}{2}(\psi_1 - \psi_2 - \psi_3 + \psi_4) = 2\begin{cases} -\sin\mu_1\xi_1 \sin\mu_2\xi_2 \exp(i\mu_3\xi_3)\,, \\ \cos\mu_1\xi_1 \cos\mu_2\xi_2 \exp(i\mu_3\xi_3)\,, \end{cases} \quad \text{for} \quad m_1 = \begin{matrix}\text{even}\,,\\ \text{odd}\,,\end{matrix}$$

$$\psi_{\mathbf{k}}^{(B_1)} = \tfrac{1}{2}(\psi_1 - \psi_2 + \psi_3 - \psi_4) = 2i\begin{cases} \sin\mu_1\xi_1 \cos\mu_2\xi_2 \exp(i\mu_3\xi_3)\,, \\ \cos\mu_1\xi_1 \sin\mu_2\xi_2 \exp(i\mu_3\xi_3)\,, \end{cases} \quad \text{for} \quad m_1 = \begin{matrix}\text{even}\,,\\ \text{odd}\,,\end{matrix}$$

$$\psi_{\mathbf{k}}^{(B_2)} = \tfrac{1}{2}(\psi_1 + \psi_2 - \psi_3 - \psi_4) = 2i\begin{cases} \cos\mu_1\xi_1 \sin\mu_2\xi_2 \exp(i\mu_3\xi_3)\,, \\ \sin\mu_1\xi_1 \cos\mu_2\xi_2 \exp(i\mu_3\xi_3)\,, \end{cases} \quad \text{for} \quad m_1 = \begin{matrix}\text{even}\,,\\ \text{odd}\,.\end{matrix} \tag{10-131}$$

where $\mu_i = 2\pi m_i$ and ψ_i are obtainable from Ψ_i in (10-128) by setting $\mathbf{p} = (0,0,0)$.

10.17.3 The star $\Sigma : \mathbf{p} = (\mathbf{p}_1, 0, 0)$.

The star Σ consists of two interior points. $\mathbf{G}_0(\mathbf{k}) = C_s = (\varepsilon, \sigma_y)$. The rep group $\mathbf{G}'_\Sigma$ is isomorphic to the point group C_s. Thus the irreps of the rep group $\mathbf{G}'_\Sigma$ are $\Delta^{(A)}(\varepsilon) = 1, \Delta^{(A)}(\sigma_y) = 1; \Delta^{(B)}(\varepsilon) = 1, \Delta^{(B)}(\sigma_y) = -1$.

The generalized projection operators $P_a^{(\mathbf{k})(\nu)b}$ are

$$P^{(\Sigma)(A)} = \tfrac{1}{2}(R_1 + R_2)\,, \quad P^{(\Sigma)(B)} = \tfrac{1}{2}(R_1 - R_2)\,, \tag{10-132}$$

where $R_1 = \{\varepsilon|0\}$, and $R_2 = \exp(i\mathbf{k}\cdot\mathbf{v})\{\sigma_y|\mathbf{v}\}$.

The irreducible basis $\psi_{\mathbf{k},a}^{(\nu)b}$ of the little group $\mathbf{G}(\Sigma)$ is

$$\psi_{\mathbf{k}}^{(A)} = \tfrac{1}{2}(R_1 + R_2)\psi_{\mathbf{k}} = \exp\{2\pi i[(p_1 + m_1)\xi_1 + m_3\xi_3]\}\begin{cases} \cos(2\pi m_2\xi_2) \\ i\sin(2\pi m_2\xi_2) \end{cases} \quad \text{for} \quad m_1 = \begin{matrix}\text{even}\,,\\ \text{odd}\,,\end{matrix}$$

$$\psi_{\mathbf{k}}^{(B)} = \tfrac{1}{2}(R_1 - R_2)\psi_{\mathbf{k}} = \exp\{2\pi i[(p_1 + m_1)\xi_1 + m_3\xi_3]\}\begin{cases} i\sin(2\pi m_2\xi_2) \\ \cos(2\pi m_2\xi_2) \end{cases} \quad \text{for} \quad m_1 = \begin{matrix}\text{even}\,,\\ \text{odd}\,.\end{matrix} \tag{10-133}$$

The irreps of the space group can be found as follows. Choose $\{\varepsilon|0\}$ and $\{C_{2z}|0\}$ as the coset representatives $\{\beta_i|\mathbf{V}(\beta_i)\}$ The $\mathbf{k}$ star is $(*\mathbf{k}) = (\mathbf{k}, -\mathbf{k})$.

Using (10-118) we can find the matrices $\mathcal{D}(\{\alpha|\mathbf{a}\})$,

$$\mathcal{D}(\{\varepsilon|0\}) = \begin{pmatrix} \Delta(\varepsilon) & \\ & \Delta(\varepsilon) \end{pmatrix}\,, \qquad \mathcal{D}(\{\sigma_x|\mathbf{v}\}) = \begin{pmatrix} & \Delta(\sigma_y) \\ \Delta(\sigma_y) & \end{pmatrix}\,,$$

$$\mathcal{D}(\{\sigma_y|\mathbf{v}\}) = \begin{pmatrix} \Delta(\sigma_y) & \\ & \Delta(\sigma_y) \end{pmatrix}\,, \quad \mathcal{D}(\{C_{2z}|\mathbf{v}\}) = \begin{pmatrix} & \Delta(\varepsilon) \\ \Delta(\varepsilon) & \end{pmatrix}\,. \tag{10-134}$$

From (10-134) and (10-120) it is trivial to obtain the irreps of C_{2v}^4. The irreducible bases $\psi_{\mathbf{k}_\sigma a}^{(\nu)b}$ of C_{2v}^4 are

$$\psi_{\mathbf{k}_1}^{(\nu)} = \psi_{\mathbf{k}}^{(\nu)}, \quad \psi_{\mathbf{k}_2}^{(\nu)} = \{C_{2z}|0\}\psi_{\mathbf{k}}^{(\nu)}, \ \nu = A, B\,. \tag{10-135}$$

10.17.4. The star $X : \mathbf{p} = (\frac{1}{2}, 0, 0)$.

The star X is a point of symmetry on the surface of the Brillouin zone: $\mathbf{G}_0(\mathbf{k}) = \mathbf{G}_o = \mathcal{C}_{2v}, q = 1$ and $\mathbf{G}(\mathbf{k}) = \mathbf{G}$. With the aid of (10-79a) we can easily find the factors $\eta(\rho, \sigma)$ and construct the group table of $\mathbf{G}'_X$, which we give in Table 10.17-2. It resembles very much Table 8.11-1, the group table for the rep group $\mathcal{D}_2^{\dagger}$. The rep group $\mathbf{G}'_X$ has $N = 5$ classes and $n = 1$ linearly independent class operator: $C_1 = R_1, C_2 = -R_1, C_3 = R_2 - R_2, C_4 = R_3 - R_3, C_5 = R_4 - R_4$. Therefore, there is only one inequivalent irrep of dimension 2, denoted by X. Choosing $C(s) = \{C_{2z}|0\}$ and diagonalizing the regular rep matrices of $C(s)$ and $\overline{C}(s)$, we obtain the eigenvectors $P_a^{(\mathbf{k})(\nu)b}$ of the CSCO-III of $\mathbf{G}'_X$ and the irreps of $\mathbf{G}'_X$, as shown in Table 10.17-3.

Table 10.17-2. Group table of $\mathbf{G}'_X$.

R_1 $\{\varepsilon\|0\}$	R_2 $\{\sigma_x\|\mathbf{v}\}'$	R_3 $\{\sigma_y\|\mathbf{v}\}'$	R_4 $\{C_{2z}\|0\}$
1	2	3	4
2	−1	−4	3
3	4	1	2
4	−3	−2	1

Table 10.17-3. Irreps of $\mathbf{G}'_X$.

	R_1	R_2	R_3	R_4
$P_1^{(X)1}$	1			1
$P_{-1}^{(X)1}$		−1	1	
$P_1^{(X)-1}$		−1	1	
$P_{-1}^{(X)-1}$	1			−1
$\Delta^{(X)}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}1&0\\1&-1\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$

The irreducible bases of $\mathbf{G}(\mathbf{k})(= \mathbf{G})$ are (ignoring the normalizations),

$$\begin{aligned} \psi_1^{(X)1} &= \psi_1 + \psi_4 , \qquad \psi_{-1}^{(X)1} = \psi_2 + \psi_3 , \\ \psi_1^{(X)-1} &= -\psi_2 + \psi_3 , \quad \psi_{-1}^{(X)-1} = \psi_1 - \psi_4 , \end{aligned} \tag{10-136}$$

where $\psi_j = R_j \psi_{\mathbf{k}}$, and are related to Ψ_j in (10-128) by

$$\psi_j = \exp[i\mathbf{k} \cdot \mathbf{V}(\gamma_j)] \Psi_j \Big|_{\mathbf{p}=(\frac{1}{2}00)} .$$

10.18. The Clebsch–Gordan Coefficients of Space Groups*

10.18.1. The CG series

Suppose that $D^{(*\mathbf{k})(\nu)}$ and $D^{(*\mathbf{k}')(\nu')}$ are two irreps of a space group $\mathbf{G}$. The Kronecker product of these two irreps can be reduced to a direct sum of the irreps of $\mathbf{G}$,

$$D^{(*\mathbf{k})(\nu)} \otimes D^{(*\mathbf{k}')(\nu')} = \sum_{*\mathbf{k}''} \sum_{\nu''} \oplus (*\mathbf{k}\nu * \mathbf{k}'\nu' | * \mathbf{k}''\nu'') D^{(*\mathbf{k}'')(\nu'')} , \tag{10-137}$$

where $(*\mathbf{k}\nu * \mathbf{k}'\nu' | * \mathbf{k}''\nu'')$ is an integer and is the number of times that the irrep $D^{(*\mathbf{k}'')(\nu'')}$ occurs in the Kronecker product rep. Equation (10-137) is referred to as the Clebsch–Gordon series of the space group, and the integer $(*\mathbf{k}\nu * \mathbf{k}'\nu' | * \mathbf{k}''\nu'')$ is called the reduction coefficient (Birman, 1974) or the multiplicity.

Several methods are available for calculating the space group reduction coefficient (Birman, 1962, 1974; Hsieh 1964; Bradley 1972). A complete and explicit set of tables for the reduction coefficients has been published (Davies, 1979, 1980; Cracknell, 1979).

Let $\psi_{\mathbf{k}_\sigma a}^{(\nu)}$ and $\psi_{\mathbf{k}'_{\sigma'} a'}^{(\nu')}$ be the basis vectors carrying the irreps $D^{(*\mathbf{k})(\nu)}$ and $D^{(*\mathbf{k}')(\nu')}$, respectively. The CG coefficients of the space group are defined as the expansion coefficients in the

following equation:

$$\psi^{(\nu'')\theta}_{\mathbf{k}_{\sigma''}a''} = \sum_{\sigma a \sigma' a'} \left[\begin{array}{c|c} \nu \mathbf{k} \nu' \mathbf{k}' & \nu'' \mathbf{k}'' \theta \\ \sigma a \sigma' a' & \sigma'' a'' \end{array}\right] \psi^{(\nu)}_{\mathbf{k}_\sigma a} \psi^{(\nu')}_{\mathbf{k}'_{\sigma'} a'} , \quad \theta = 1, 2, \ldots, (*\mathbf{k}\nu * \mathbf{k}'\nu' | * \mathbf{k}''\nu'') , \quad (10\text{-}138)$$

where θ is the multiplicity label. The inverse of (10-138) is

$$\psi^{(\nu)}_{\mathbf{k}_\sigma a} \psi^{(\nu')}_{\mathbf{k}'_{\sigma'} a'} = \sum_{\nu'' \mathbf{k}'' \sigma'' a'' \theta} \left[\begin{array}{c|c} \nu \mathbf{k} \nu' \mathbf{k}' & \nu'' \mathbf{k}'' \theta \\ \sigma a \sigma' a' & \sigma'' a'' \end{array}\right] \psi^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''} a''} . \quad (10\text{-}139a)$$

The CG coefficients can also be written as

$$\left[\begin{array}{c|c} \nu \mathbf{k} \nu' \mathbf{k}' & \nu'' \mathbf{k}'' \theta \\ \sigma a \sigma' a' & \sigma'' a'' \end{array}\right] = \langle \psi^{(\nu)}_{\mathbf{k}_\sigma a} \psi^{(\nu')}_{\mathbf{k}'_{\sigma'}, a'} | \psi^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''} a''} \rangle . \quad (10\text{-}139b)$$

With the aid of

$$\begin{aligned} \langle \psi^{(\nu)}_{\mathbf{k}_\sigma a} \psi^{(\nu')}_{\mathbf{k}'_{\sigma'} a'} | \{\varepsilon | \mathbf{R}_n\} | \psi^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''} a''} \rangle &= \exp(-i\mathbf{k}''_{\sigma''} \cdot \mathbf{R}_n) C \\ &= \langle \{\varepsilon | -\mathbf{R}_n\} (\psi^{(\nu)}_{\mathbf{k}_\sigma a} \psi^{(\nu')}_{\mathbf{k}'_{\sigma'} a'}) | \psi^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''} a''} \rangle = \exp(-(\mathbf{k}_\sigma + \mathbf{k}'_{\sigma'}) \cdot \mathbf{R}_n) C , \end{aligned}$$

where C is the abbreviation for the CG coefficient (10-139b), we know that the CG coefficient vanishes unless

$$\mathbf{k}_\sigma + \mathbf{k}'_{\sigma'} - \mathbf{k}''_{\sigma''} = \mathbf{K}_m . \quad (10\text{-}140)$$

According to (10-140) we can introduce the wave-vector selection rule,

$$*\mathbf{k} \otimes *\mathbf{k}' = \sum_{*\mathbf{k}''} (*\mathbf{k} * \mathbf{k}' | * \mathbf{k}'') * \mathbf{k}'' . \quad (10\text{-}141)$$

The integers $(*\mathbf{k} * \mathbf{k}' | * \mathbf{k}'')$ are referred to as the wave vector reduction coefficients. They satisfy

$$(*\mathbf{k} * \mathbf{k}' | * \mathbf{k}'') = (*\mathbf{k}' * \mathbf{k} | * \mathbf{k}'') . \quad (10\text{-}142)$$

Assuming that there are q, q', and q'' points in the stars $*\mathbf{k}, *\mathbf{k}'$ and $*\mathbf{k}''$, respectively, it follows from (10-141) that

$$qq' = \sum_{*\mathbf{k}''} (*\mathbf{k} * \mathbf{k}' | * \mathbf{k}'') q'' . \quad (10\text{-}143a)$$

A simple prescription for determining the wave vector reduction coefficients is given by Birman (1962) and is reproduced here.

The $q \cdot q'$ wave vectors $\mathbf{k}_\sigma + \mathbf{k}'_\tau$ can be expressed as

$$\beta_\sigma(k + \mathbf{k}'_{\sigma'}) = \beta_\sigma(\mathbf{k} + \beta_{\sigma'} \mathbf{k}') , \quad \sigma = 1, 2, \ldots, q; \quad \sigma' = 1, 2, \ldots, q' . \quad (10\text{-}143b)$$

Let us introduce a table, called the wave vector table, the entry of which in the σ–th row and σ'–th column is $\beta_\sigma(\mathbf{k} + \beta_{\sigma'} \mathbf{k}')$. Suppose that $\mathbf{k} + \beta_{\sigma'} \mathbf{k}'$ belongs to the star $*\mathbf{k}''$, then $\beta_\sigma(\mathbf{k} + \beta_{\sigma'} \mathbf{k}')$ still belongs to the star $*\mathbf{k}''$. In other words, all the wave vectors in the wave vector table belong to the same star. Therefore, to determine the wave vector selection rule, it suffices to construct a single row, say the first row, of the wave vector table. From this row and using (10-143a) we can obtain the wave vector selection rule. It is convenient to choose $q \geq q'$, that is, let the number of rows be larger than or equal to the number of columns in the wave vector table. As examples, we consider the selection rules for the face–centered cubic lattice Γ^f_c.

Example 1: $W(\frac{1}{2}, \frac{1}{4}, \frac{3}{4}) \otimes X(\frac{1}{2}, 0, \frac{1}{2})$. According to Table 3.11 in Bradley (1972, pp. 162), $q = q_W = 6, q' = q_X = 3$. The star X consists of three points: $\mathbf{k}'_{\sigma'} = (\frac{1}{2} 0 \frac{1}{2})$, $(\frac{1}{2} \frac{1}{2} 0)$, and $(0 \frac{1}{2} \frac{1}{2})$.

Using (10-140) we can construct Table 10.18-1. Consulting Bradley's Table 3.11, we know that $\mathbf{k}_\Delta = (0\frac{1}{4}\frac{1}{4})$ and $q'' = q_\Delta = 6$. Therefore, we have the selection rule

$$*W \otimes *X = 2 * \Delta + *W \ . \tag{10-143c}$$

Example 2: $\Delta(\alpha 0\alpha) \otimes X(\frac{1}{2}0\frac{1}{2})$ $(\alpha \leq \frac{1}{2})$. $q = q_\Delta = 6, q' = q_X = 3$. Similarly, from Table 10.18-2, Eq. (10-143a) and $q'' = q_Z = 12$, we get

$$*\Delta \otimes *X = *\Delta' + *Z \ . \tag{10-143d}$$

Table 10.18-1. Wave vector table for $*W \otimes *X$.

q \ q'	1	2	3
1	Δ $(0, \frac{1}{4}, \frac{1}{4})$	Δ $(0, \frac{3}{4}, \frac{3}{4})$	W $(\frac{1}{2}, \frac{3}{4}, \frac{1}{2})$

Table 10.18-2. Wave vector table for $*\Delta \otimes *X$.

q \ q'	1	2	3
1	Δ' $(\frac{1}{2}+\alpha, 0, \frac{1}{2}+\alpha)$	Z $(\frac{1}{2}+\alpha, \frac{1}{2}, \alpha)$	Z $(\alpha, \frac{1}{2}, \frac{1}{2}+\alpha)$

10.18.2. The calculation of the CG coefficients

Setting $\sigma'' = 1$ in (10-138), we have

$$\psi^{(\nu'')\theta}_{\mathbf{k}''a''} = \sum_{\sigma a \sigma' a'} \left[\begin{matrix} \nu \mathbf{k} \nu' \mathbf{k}' \\ \sigma a \sigma' a' \end{matrix} \middle| \begin{matrix} \nu'' \mathbf{k}'' \theta \\ 1 a'' \end{matrix} \right] |\sigma a \sigma' a'\rangle \ , \tag{10-144a}$$

where

$$|\sigma a \sigma' a'\rangle \equiv \psi^{(\nu)}_{\mathbf{k}_\sigma a} \psi^{(\nu')}_{\mathbf{k}'_{\sigma'} a'} \ . \tag{10-144b}$$

Since $\psi^{(\nu'')\theta}_{\mathbf{k}''a''}$ is the irreducible basis of the rep group $\mathbf{G}'_{\mathbf{k}''}$, it is necessarily an eigenvector of the CSCO-II $(C, C(s))$ of the group $\mathbf{G}'_{\mathbf{k}''}$:

$$\begin{pmatrix} C \\ C(s) \end{pmatrix} \psi^{(\nu'')\theta}_{\mathbf{k}''a''} = \begin{pmatrix} \nu'' \\ a'' \end{pmatrix} \psi^{(\nu'')\theta}_{\mathbf{k}''a''} \ , \tag{10-145a}$$

or, written in matrix form

$$\begin{pmatrix} M(C) \\ M(C(s)) \end{pmatrix} U^{(\nu'')\theta}_{\mathbf{k}''a''} = \begin{pmatrix} \nu'' \\ a'' \end{pmatrix} U^{(\nu'')\theta}_{\mathbf{k}''a''} \ , \tag{10-145b}$$

where $M(C)$ and $M(C(s))$ are the representatives of the operators C and $C(s)$ in the uncoupled representation with the basis $|\sigma a \sigma' a'\rangle$, and the vector

$$U^{(\nu'')\theta}_{\mathbf{k}''a''} = \left\{ \left[\begin{matrix} \nu \mathbf{k} \nu' \mathbf{k}' \\ \sigma a \sigma' a' \end{matrix} \middle| \begin{matrix} \nu'' \mathbf{k}'' \theta \\ 1 a'' \end{matrix} \right] \right\} \tag{10-146}$$

is the representative of $\psi^{(\nu'')\theta}_{\mathbf{k}''a''}$; (ν'', a'') is the eigenvalue of $(C, C(s))$. In other words, the CG coefficients (10-146) result from a diagonalization of the matrices $M(C)$ and $M(C(s))$ simultaneously. To calculate $M(C)$ and $M(C(s))$, we must first calculate the matrices $M(\{\gamma''|\mathbf{c}''\})$ for the group elements $\{\gamma''|\mathbf{c}''\}'$ contained in the CSCO–II of $\mathbf{G}'_{\mathbf{k}''}$. In this section, to avoid notational clumsiness, we use the abbreviation

$$\{\gamma''|\mathbf{c}''\} \equiv \{\gamma''|\mathbf{V}(\gamma'')\} \,. \tag{10-147}$$

From $\{\gamma''|\mathbf{c}''\}' = \exp(i\mathbf{k}'' \cdot \mathbf{c}'')\{\gamma''|c''\}$, we have

$$M(\{\gamma''|\mathbf{c}''\}') = \exp(i\mathbf{k}'' \cdot \mathbf{c}'')M(\{\gamma''|\mathbf{c}''\}) \,. \tag{10-148}$$

The matrix elements of $M(\{\gamma''|\mathbf{c}''\})$ can be expressed as

$$\begin{aligned} M_{\tau b\tau' b',\sigma a\sigma' a'}(\{\gamma''|\mathbf{c}''\}) &= \langle \tau b\tau' b'|\{\gamma''|\mathbf{c}''\}|\sigma a\sigma' a'\rangle \\ &= D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}(\{\gamma''|\mathbf{c}''\}) D^{(*\mathbf{k}')(\nu')}_{\tau' b',\sigma' a'}(\{\gamma''|\mathbf{c}''\}) \,, \end{aligned} \tag{10-149a}$$

or in the form of a direct product of the matrices

$$M(\{\gamma''|\mathbf{c}''\}) = D^{(*\mathbf{k})(\nu)}(\{\gamma''|\mathbf{c}''\}) \otimes D^{(*\mathbf{k}')(\nu')}(\{\gamma''|\mathbf{c}''\}) \,. \tag{10-149b}$$

The matrices $D^{(*\mathbf{k})(\nu)}(\{\gamma''|\mathbf{c}''\})$ and $D^{(*\mathbf{k}')(\nu')}(\{\gamma''|\mathbf{c}''\})$ can be evaluated from the irreps of the rep groups $\mathbf{G}'_{\mathbf{k}}$ and $\mathbf{G}'_{\mathbf{k}'}$ using (10-114) or (10-120), while the matrices $M(C)$ and $M(C(s))$ can be evaluated by using Eq. (10-149). From the secular equations of $M(C)$ and $M(C(s))$, we can get the eigenvalues $(\nu''a'')$ and their degeneracies. If the degeneracy of the eigenvalue $(\nu''a'')$ is d, the reduction coefficient is

$$(*\mathbf{k}\nu * \mathbf{k}'\nu' | * \mathbf{k}''\nu'') = d \,. \tag{10-150}$$

Substituting the eigenvalue (ν'', a'') into (10-145b), we can get d orthogonal eigenvectors,

$$U^{(\nu'')\theta}_{\mathbf{k}''a''} = \left\{ \left[\begin{array}{c|c} \nu\mathbf{k}\nu'\mathbf{k}' & \nu''\mathbf{k}''\theta \\ \sigma a\sigma' a' & 1a'' \end{array} \right] \right\} \,, \quad \theta = 1, 2, \ldots, d \,, \tag{10-151}$$

where the component index for the vector U is $(\sigma a\sigma' a')$.

10.18.3. Relative phase of the CG coefficients

To ensure that the CG coefficients (10-146) with the same ν'', $\mathbf{k}''$, and θ, but different a'' have the correct relative phase, we can use the following technique.

Suppose that we have found d orthogonal eigenvectors $U^{(\nu'')\theta}_{\mathbf{k}''a''}, \theta = 1, 2, \ldots d$, for a particular a''. To find the CG vector for the component b'', we search for an element $R_i = \{\gamma_i|\mathbf{v}_i\}'$ of $G'_{\mathbf{k}''}$ which has only one non–vanishing element in the a''–th column of the ν''–th irrep,

$$R_i \psi^{(\nu'')}_{\mathbf{k}''a''} = \Delta_{a''a''}(\gamma_i)\psi^{(\nu'')}_{\mathbf{k}''a''} + \Delta_{b''a''}(\gamma_i)\psi^{(\nu'')}_{\mathbf{k}''b''} \,. \tag{10-152}$$

Then we have

$$U^{(\nu'')\theta}_{\mathbf{k}''b''} = [\Delta_{b''a''}(\gamma_i)]^{-1}[M(R_i) - \Delta_{a''a''}(\gamma_i)]U^{(\nu'')\theta}_{\mathbf{k}''a''} \,. \tag{10-153}$$

By choosing in each step appropriate R_i's which obey the condition (10-152), all the other eigenvectors $U^{(\nu'')}_{\mathbf{k}''b''}$ can be found in turn from (10-153). In a few cases for given a'' and b'' we cannot find an element satisfying (10-153). For such cases, we search for two elements R_i and R_j which only have two non–vanishing off diagonal elements in the a''–th column of ν''–th irrep, that is,

$$\begin{aligned} R_i\psi_{a''} &= \Delta_{a''a''}(\gamma_i)\psi_{a''} + \Delta_{b''a''}(\gamma_i)\psi_{b''} + \Delta_{c''a''}(\gamma_i)\psi_{c''} \,, \\ R_j\psi_{a''} &= \Delta_{a''a''}(\gamma_j)\psi_{a''} + \Delta_{b''a''}(\gamma_j)\psi_{b''} + \Delta_{c''a''}(\gamma_j)\psi_{c''} \,, \end{aligned} \tag{10-154}$$

where obvious shorthand notation is used. Solving the linear equations (10-154), we can find both $\psi_{b''}$ and $\psi_{c''}$ from $\psi_{a''}$. This process can be extended further, however in practice Eqs. (10-153) and (10-154) are sufficient.

10.18.4. The full CG coefficients of space groups

Up to now we have found only the CG coefficients $U^{(\nu'')\theta}_{\mathbf{k}''a''}$ corresponding to $\sigma'' = 1$. It follows from (10-106) that the CG coefficients

$$U^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''}a''} = \left\{ \left[\begin{array}{c|c} \nu\mathbf{k}\nu'\mathbf{k}' & \nu''\mathbf{k}''\theta \\ \sigma a\sigma' a' & \sigma'' a'' \end{array} \right] \right\} \tag{10-155}$$

for $\sigma'' \neq 1$ can be found from $U^{(\nu'')\theta}_{\mathbf{k}''a''}$ by the formula

$$\begin{aligned} U^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''}a''} &= M(\{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\})U^{(\nu'')\theta}_{\mathbf{k}''a''} \\ &= D^{(*\mathbf{k})(\nu)}(\{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\}) \otimes D^{(*\mathbf{k}')(\nu')}(\{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\})U^{(\nu'')\theta}_{\mathbf{k}''a''} , \end{aligned} \tag{10-156}$$

where $\{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\}$ is the coset representative of the space group $\mathbf{G}$ with respect to the little group $\mathbf{G}(\mathbf{k}'')$:

$$\mathbf{G} = \sum_{\sigma''=1}^{q''} \{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\}\mathbf{G}(\mathbf{k}'') . \tag{10-157}$$

Equation (10-156) can be rewritten as

$$\left[\begin{array}{c|c} \nu\mathbf{k}\nu'\mathbf{k}' & \nu''\mathbf{k}''\theta \\ \tau b\tau' b' & \sigma'' a'' \end{array} \right] = \sum_{aa'} D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}(\{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\}) D^{(*\mathbf{k}')(\nu')}_{\tau' b',\sigma' a'}(\{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\}) \left[\begin{array}{c|c} \nu\mathbf{k}\nu'\mathbf{k}' & \nu''\mathbf{k}''\theta \\ \sigma a\sigma' a' & 1a'' \end{array} \right] . \tag{10-158}$$

Observe that there is no summation over σ and σ' on the right-hand side of (10-158), since the index $\sigma(\sigma')$ is uniquely specified by $\tau(\tau')$ and $\{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\}$, for which the submatrix

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\})\left[D^{(*\mathbf{k}')(\nu')}_{(\tau'\sigma')}(\{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\})\right]$$

does not vanish.

Some remarks:

The following remarks should be added in regard to the eigenfunction method for evaluating CG coefficients of space groups.

1. Here we only need to know *a priori* the wave vector selection rule (which is easy to work out), but not the CG series.

2. For computer calculations, the CSCO–II of $\mathbf{G}'_{\mathbf{k}''}$ can be appropriately chosen so that it consists of only a single operator.

3. It seems at first sight that the order of the eigenequation (10-145b) is equal to $(qh_\nu) \times (q'h_{\nu'})$. But actually, due to the wave vector selection rule (10-140), the order of (10-145b) is much smaller.

10.18.5. A summary of the eigenfunction method for space group CG coefficients

The scheme for obtaining the CG coefficients of space groups can be summarized as follows.

1. Determine the wave vector selection rule.

2. Pick out one star $*\mathbf{k}''$ among those stars for which the wave vector reduction coefficients $(*\mathbf{k} * \mathbf{k}'| * \mathbf{k}'') \geq 1$ and its CG coefficients are to be calculated.

3. Choose the canonical wave vectors $\mathbf{k}, \mathbf{k}'$, and $\mathbf{k}''$.

4. For each of the canonical wave vectors, choose appropriate coset representatives of $\mathbf{G}$,

$$\begin{aligned}\mathbf{G} &= \sum_{\sigma} \oplus \{\beta_\sigma | \mathbf{V}_\sigma\} \mathbf{G}(\mathbf{k}) \ , \quad \mathbf{G} = \sum_{\sigma'} \oplus \{\beta_{\sigma'} | \mathbf{V}_{\sigma'}\} \mathbf{G}(\mathbf{k}') \ , \\ \mathbf{G} &= \sum_{\sigma''} \oplus \{\beta'' | \mathbf{V}_{\sigma''}\} \mathbf{G}(\mathbf{k}'') \ ,\end{aligned} \tag{10-159}$$

and find all the $\mathbf{k}$ points in the stars $*\mathbf{k}$ and $*\mathbf{k}'$ according to

$$\begin{aligned}\mathbf{k}_\sigma &= \beta_\sigma \mathbf{k} \ , \qquad \sigma = 1, 2, \ldots, q \ , \\ \mathbf{k}'_{\sigma'} &= \beta_{\sigma'} \mathbf{k}' \ , \quad \sigma' = 1, 2, \ldots, q' \ .\end{aligned} \tag{10-160}$$

To simplify the calculation, in the following we always choose as the coset representatives elements whose non-primitive translations are zero, that is, we assume

$$\mathbf{V}_\sigma = \mathbf{V}_{\sigma'} = \mathbf{V}_{\sigma''} = 0 \ . \tag{10-161}$$

5. Determine all the index pairs $(\sigma\sigma')$ which satisfy

$$\mathbf{k}_\sigma + \mathbf{k}'_{\sigma'} = \mathbf{k}'' + \mathbf{K}_m \ . \tag{10-162}$$

For convenience in exposition, we assume in the following that there exist only two such pairs $(\sigma\sigma')$ and $(\tau\tau')$.

6. Using the eigenfunction method or consulting an existing table, for example, the Kovalev (1961) table, find the irreps $D^{(\mathbf{k})(\nu)}, D^{(\mathbf{k}')(\nu')}$ and $D^{(\mathbf{k}'')(\nu'')}$ for the rep groups $\mathbf{G}_\mathbf{k}, \mathbf{G}_{\mathbf{k}'}$, and $\mathbf{G}_{\mathbf{k}''}$, respectively.

7. Construct the irreducible matrices $D^{(*\mathbf{k})(\nu)}(\{\gamma''|\mathbf{V}(\gamma'')\})$ and $D^{(*\mathbf{k}')(\nu')}(\{\gamma''|\mathbf{V}(\gamma'')\})$ for the elements $\{\gamma''|\mathbf{V}(\gamma'')\}$ of the group $\mathbf{G}_{\mathbf{k}''}$, from which the CSCO-II of $\mathbf{G}_{\mathbf{k}''}$ is composed. However, only the submatrices related to the indices $\sigma, \tau, (\sigma', \tau')$, instead of the full matrices $D^{(*\mathbf{k})(\nu)}(D^{(*\mathbf{k}')(\nu')})$, are required to determine the CG coefficients, for example,

$$\left[D^{(*\mathbf{k})(\nu)}(\{\gamma''|\mathbf{V}(\gamma'')\})\right] = \begin{array}{c} \\ \tau \\ \sigma \end{array} \begin{array}{c} \begin{array}{cc} \tau & \sigma \end{array} \\ \begin{pmatrix} D_{(\tau\tau)} & D_{(\tau\sigma)} \\ D_{(\sigma\tau)} & D_{(\sigma\sigma)} \end{pmatrix} \end{array}$$

$$\left[D^{(*\mathbf{k}')(\nu')}(\{\gamma''|\mathbf{V}(\gamma'')\})\right] = \begin{array}{c} \\ \tau' \\ \sigma' \end{array} \begin{array}{c} \begin{array}{cc} \tau' & \sigma' \end{array} \\ \begin{pmatrix} D'_{(\tau'\tau')} & D'_{(\tau'\sigma')} \\ D'_{(\sigma'\tau')} & D'_{(\sigma'\sigma')} \end{pmatrix} \end{array} , \tag{10-163a}$$

where the large square brackets denote a submatrix, and

$$\begin{aligned}D_{(\tau\sigma)} &= \exp[-i\mathbf{k}_\tau \cdot \mathbf{V}(\gamma'')] \Delta(\beta_\tau^{-1} \gamma'' \beta_\sigma) \ , \\ D'_{(\tau'\sigma')} &= \exp[-i\mathbf{k}'_{\tau'} \cdot \mathbf{V}(\gamma'')] \Delta(\beta_{\tau'}^{-1} \gamma'' \beta_{\sigma'}) \ ,\end{aligned} \tag{10-163b}$$

from Eq. (10-120).

8. With the help of Eq. (10-149b), construct the representation matrix of $\{\gamma''|\mathbf{V}(\gamma'')\}$ in the uncoupled rep,

$$M(\{\gamma''|\mathbf{V}(\gamma'')\}') = \begin{array}{c} \\ \tau\tau' \\ \sigma\sigma' \end{array} \begin{array}{c} \begin{array}{cc} \tau\tau' & \sigma\sigma' \end{array} \\ \begin{pmatrix} D_{(\tau\tau)} \otimes D'_{(\tau'\tau')} & D_{(\tau\sigma)} \otimes D'_{(\tau'\sigma')} \\ D_{(\sigma\tau)} \otimes D'_{(\sigma'\tau')} & D_{(\sigma\sigma)} \otimes D'_{(\sigma'\sigma')} \end{pmatrix} \end{array} . \tag{10-164a}$$

Then form the matrix

$$M(\{\gamma''|\mathbf{V}(\gamma'')\}') = \exp[i\mathbf{k}''\cdot\mathbf{V}(\gamma'')]M(\{\gamma''|\mathbf{V}(\gamma'')\}) \ . \tag{10-164b}$$

The ordering for rows or columns in the matrix M is as follows:

$$\begin{aligned} &|\tau 1\tau' 1\rangle \ldots |\tau 1\tau' h_{\nu'}\rangle, |\tau 2\tau' 1\rangle \ldots |\tau 2\tau' h_{\nu'}\rangle \ldots |\tau h_\nu \tau' h_{\nu'}\rangle \ , \\ &|\sigma 1\sigma' 1\rangle \ldots |\sigma 1\sigma' h_{\nu'}\rangle, |\sigma 2\sigma' 1\rangle \ldots |\sigma 2\sigma' h_{\nu'}\rangle \ldots |\sigma h_\nu \sigma' h_{\nu'}\rangle \ . \end{aligned} \tag{10-165}$$

Suppose the class operator C_i is contained in the CSCO–II of $\mathbf{G}'_{\mathbf{k}''}$. By adding up the matrices $M(\{\gamma''|\mathbf{V}(\gamma'')\}')$ for all $\{\gamma''|\mathbf{V}(\gamma'')\}'$ belonging to the class i, we obtain the matrix $M(C_i)$. In this way we can obtain the matrices $M(C)$ and $M(C(s))$ of the CSCO–II of $\mathbf{G}'_{\mathbf{k}''}$.

9. By diagonalizing the matrices $M(C)$ and $M(C(s))$ simultaneously, we get the eigenvalues $(\nu''a'')$ and their degeneracies $d = (*\mathbf{k}\nu * \mathbf{k}'\nu' | * \mathbf{k}''\nu'')$. Or equivalently, we first diagonalize the matrix $M(C)$ and get the eigenvalues ν'' and the corresponding degeneracies $m_{\nu''}$. Then the reduction coefficient $(*\mathbf{k}\nu * \mathbf{k}'\nu' | * \mathbf{k}''\nu'') = m_{\nu''}/h_{\nu''}; h_{\nu''}$ is the dimension of the irrep $D^{(\mathbf{k}'')(\nu'')}$ of $\mathbf{G}'_{\mathbf{k}''}$.

For each ν'' and a specific but arbitrarily chosen a'', find the eigenvectors $U^{(\nu'')\theta}_{\mathbf{k}''a''}, \theta = 1, 2, \ldots, d$.

10. Using (10-154), obtain all the CG coefficients belonging to $\sigma'' = 1$.

11. Using (10-158), obtain the CG coefficients for $\sigma'' \neq 1$.

12. Pick out another star $*\mathbf{k}''$, choose its canonical wave vector $\mathbf{k}''$ and coset representatives $\{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\}$, then return to step 5 and go through to the end.

10.19. Examples: Getting Space Group Clebsch–Gordan Coefficients*

In this section, following the prescription in Sec. 10.18, we shall give two examples of calculations for the CG coefficients of the non–symmorphic space group O_h^7.

10.19.1. The CG coefficients of O_h^7 for $*X(1) \otimes *X(2) \to *X(\nu'')$

1. The wave vector selection rule is easily found:

$$*X \otimes *X = 3\Gamma + 2 * X \ . \tag{10-166}$$

2. Pick out $*\mathbf{k}'' = *X$.

3. The canonical wave vectors are chosen as

$$\mathbf{k} = \mathbf{k}' = \mathbf{k}'' = \mathbf{k}_z = \left(\tfrac{1}{2}, \tfrac{1}{2}, 0\right) \ , \tag{10-167}$$

with $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ as basis.

Notice that the choice in (10-167) is different from that given by Berenson, (1975). They choose

$$\mathbf{k} = \mathbf{k}_x, \quad \mathbf{k}' = \mathbf{k}_y, \quad \mathbf{k}'' = \mathbf{k}_z \ . \tag{10-168}$$

4. The coset representatives of O_h^7 with respect to the little group $\mathbf{G}(X)$ are chosen to be

$$\{\beta_2|\mathbf{V}_2\} = \{C_{31}^+|0\} \ , \quad \{\beta_3|\mathbf{V}_3\} = \{C_{31}^-|0\} \ . \tag{10-169}$$

Under the rotation C_{31}^+, the wave vectors $\mathbf{k}_x, \mathbf{k}_y$ and $\mathbf{k}_z$ transform among themselves cyclically.

The star X contains three $\mathbf{k}$ points, $\mathbf{k}_\sigma = \beta_\sigma \mathbf{k}$,

$$\mathbf{k}_1 = \mathbf{k} = \mathbf{k}_z = \left(\tfrac{1}{2}, \tfrac{1}{2}, 0\right) \ , \quad \mathbf{k}_2 = \mathbf{k}_x = \left(0, \tfrac{1}{2}, \tfrac{1}{2}\right) \ , \quad \mathbf{k}_3 = \mathbf{k}_y = \left(\tfrac{1}{2}, 0, \tfrac{1}{2}\right) \ . \tag{10-170}$$

5. From (10-170) it is readily seen that

$$\mathbf{k}_x + \mathbf{k}_y = \mathbf{k}_z + (001) \,. \tag{10-171}$$

Hence the index pairs are $(\tau\tau') = (23)$ and $(\sigma\sigma') = (32)$.

6. The ray or projective irreps $\Delta^{X_i}(\gamma)$ for the little co-group $\mathbf{G}_0(\mathbf{X})$ are given in Kovalev (1961, Table T159). We list them here in Table 10.19-1. In Table 10.19-1 and in the following we often use the symbols

$$\varepsilon = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \quad \lambda = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \quad \varphi = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \kappa = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} , \mu = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} . \tag{10-172}$$

7. From Eq.(10-101) we know that the CSCO–I of the group $\mathbf{G}'_X$ is

$$C = (C_1, C_2) \,, \quad C_1 = \{C_{2a}|\tau\}' - \{C_{2b}|\tau\}' \,, C_2 = \{\sigma_{da}|0\} + \{\sigma_{ab}|0\} \,. \tag{10-173}$$

The eigenvalues of (C_1, C_2) are listed in Table 10.19-1. Furthermore, from this table it is seen that apart from the identity the only elements whose matrices are always diagonalized for the irreps $X_1 - X_4$ are $\{C_{4z}^+|\boldsymbol{\tau}\}'$ and $\{C_{4z}^-|\tau\}'$. Hence either $\{C_{4z}^+|\tau\}'$ or $\{C_{4z}^-|\tau\}'$ can be taken as the operator $C(s)$, whose eigenvalues are used to distinguish the two basis vectors of the irreps $X_1 - X_4$. We choose

$$C(s) = \{C_{4z}^+|\tau\}' \,. \tag{10-174}$$

The eigenvalues of $C(s)$ listed in Table 10.19-1 are inferred from the diagonal elements of the matrices $\Delta^{X_j}(C_{4z}^+)$.

Using (10-114) or (10-163) and Table 10.19-1 we can easily construct the space group rep $D^{(*X)(\nu)}$. For example,

$$\mathcal{D}(\{C_{4z}^+|\boldsymbol{\tau}\}) = \begin{array}{c} \\ \varepsilon \\ C_{31}^- \\ C_{31}^+ \end{array} \begin{array}{c} \begin{array}{ccc} \varepsilon & C_{31}^+ & C_{31}^- \end{array} \\ \begin{pmatrix} \Delta(C_{4z}^+) & 0 & 0 \\ 0 & 0 & \Delta(C_{2a}) \\ 0 & \Delta(C_{4z}^-) & 0 \end{pmatrix} \end{array} , \tag{10-175a}$$

$$\begin{aligned} D^{(*X)(j)}(\{C_{4z}^+|\boldsymbol{\tau}\}) &= -i\mathcal{D}(\{C_{4z}^+|\tau\}) \\ &= \begin{pmatrix} -\lambda i & 0 & 0 \\ 0 & 0 & -\kappa i \\ 0 & -\lambda i & 0 \end{pmatrix} , \quad j = 1, 2 \,. \end{aligned} \tag{10-175b}$$

Similarly we have

$$D^{(*X)(j)}(\{C_{2a}|\tau\}) = \begin{pmatrix} -\kappa i & 0 & 0 \\ 0 & 0 & -\lambda i \\ 0 & -\lambda i & 0 \end{pmatrix} ,$$

$$D^{(*X)(j)}(\{C_{2b}|\tau\}) = \begin{pmatrix} -\kappa i & 0 & 0 \\ 0 & 0 & -\kappa i \\ 0 & -\kappa i & 0 \end{pmatrix} , \tag{10-175c}$$

$$D^{(*X)(j)}(\{\sigma_{da}|0\}) = (-1)^{j+1} \begin{pmatrix} \varepsilon & 0 & 0 \\ 0 & 0 & \varphi \\ 0 & \varphi & 0 \end{pmatrix} ,$$

$$D^{(*X)(j)}(\{\sigma_{db}|0\}) = (-1)^{j+1} \begin{pmatrix} \varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix} , \quad j = 1, 2 \,.$$

Table 10.19-1. The ray irreps $\Delta^{X_i}(\gamma)$ for the little co-group $\mathbf{G}_0(\mathbf{X})$. That is, the irreps of the rep group $\mathbf{G}'_X$. $\Delta^{X_2} = \delta^{(2)}\Delta^{X_1}$, $\Delta^{X_4} = \delta^{(4)}\Delta^{X_3}$; $X_1 \to \hat{\tau}^3$, $X_2 \to \hat{\tau}^4$, $X_3 \to \hat{\tau}^2$, $X_4 \to \hat{\tau}^1$, where $\hat{\tau}^i$ are the labels used by Kovalev. This table is taken from Kovalev (1961).

	(C_1, C_2)	$C(s)$	ϵ	C_{2y}	C_{2z}	C_{2x}	C_{4z}^-	C_{4z}^+	C_{2a}	C_{2b}	I	σ_y	σ_z	σ_x	S_{4z}^+	S_{4z}^-	σ_{da}	σ_{db}	
X_1	$(0,2)$	$\begin{pmatrix} 1 \\ -1 \end{pmatrix}$		ϵ	φ	ϵ	φ	λ	λ	κ	κ	κ	λ	κ	λ	φ	φ	ϵ	ϵ
X_2	$(0,-2)$	$\begin{pmatrix} 1 \\ -1 \end{pmatrix}$	$\delta^{(2)}$	$+$	$+$	$+$	$+$	$+$	$+$	$+$	$+$	$-$	$-$	$-$	$-$	$-$	$-$	$-$	$-$
X_3	$(2i,0)$	$\begin{pmatrix} -i \\ i \end{pmatrix}$		ϵ	λ	$-\epsilon$	$-\lambda$	λi	$-\lambda i$	ϵi	$-\epsilon i$	κ	$-\varphi$	$-\kappa$	φ	φi	$-\varphi i$	$-\kappa i$	κi
X_4	$(-2i,0)$	$\begin{pmatrix} -i \\ i \end{pmatrix}$	$\delta^{(4)}$	$+$	$-$	$+$	$-$	$+$	$+$	$-$	$-$	$+$	$-$	$+$	$-$	$+$	$+$	$-$	$-$

Table 10.19-2. The CG coefficients $\left(\begin{array}{c|c} \nu\mathbf{k}\nu'\mathbf{k}' & X(j) \\ \sigma a \sigma' a' & k_z a'' \end{array}\right)$ of O_h^7 for $*X(1) \otimes *X(2)$ and $\sigma'' = 1$. We use, for example, $xayb$ to signify $k_x a k_y b$.

	(C_1, C_2)	$C(s)$	N	$x1y1$	$x1y2$	$x2y1$	$x2y2$	$y1x1$	$y1x2$	$y2x1$	$y2x2$
$X(1)$	$(0,2)$	1	$\sqrt{\frac{1}{8}}$	1	$-i$	$-i$	1	-1	i	i	-1
		-1	$\sqrt{\frac{1}{8}}$	$-i$	1	1	$-i$	i	-1	-1	i
$X(2)$	$(0,-2)$	1	$\sqrt{\frac{1}{8}}$	1	i	i	1	1	i	i	1
		-1	$\sqrt{\frac{1}{8}}$	i	1	1	i	i	1	1	i
$X(3)$	$(2i,0)$	$-i$	$\sqrt{\frac{1}{8}}$	1	-1	1	-1	-1	-1	1	1
		i	$\sqrt{\frac{1}{8}}$	i	i	$-i$	$-i$	$-i$	i	$-i$	i
$X(4)$	$(-2i,0)$	$-i$	$\sqrt{\frac{1}{8}}$	1	1	-1	-1	1	-1	1	-1
		i	$\sqrt{\frac{1}{8}}$	i	$-i$	i	$-i$	i	i	$-i$	$-i$

8. From (10-164) and (10-175) we have

$$M(C_1) = M(\{C_{2a}|\tau\}') - M(\{C_{2b}|\tau\}') = \begin{array}{c} \\ 23 \\ \\ \\ 32 \end{array} \begin{array}{c} \begin{array}{cccc} 23 & & 32 & \end{array} \\ \begin{pmatrix} & & -\lambda & \kappa \\ & & -\kappa & \lambda \\ -\lambda & \kappa & & \\ -\kappa & \lambda & & \end{pmatrix} \end{array} \times (i) \ , \tag{10-176a}$$

$$M(C_2) = -\begin{pmatrix} & & \varepsilon & \varphi \\ & & \varphi & \varepsilon \\ \varepsilon & \varphi & & \\ \varphi & \varepsilon & & \end{pmatrix} , \qquad M(C(s)) = i\begin{pmatrix} & & 0 & \lambda \\ & & -\lambda & 0 \\ \kappa & 0 & & \\ 0 & -\kappa & & \end{pmatrix} , \tag{10-176b}$$

$$M(\{C_{2a}|\tau\}') = i\begin{pmatrix} & & -\lambda & 0 \\ & & 0 & \lambda \\ -\lambda & 0 & & \\ 0 & \lambda & & \end{pmatrix} , \quad M(\{\sigma_a|0\}) = \begin{pmatrix} & & 0 & \varphi \\ & & \varphi & 0 \\ 0 & \varphi & & \\ \varphi & 0 & & \end{pmatrix} . \tag{10-176c}$$

By setting $(\tau\tau') = (23), (\sigma\sigma') = (32)$, and $h_\nu = h_{\nu'} = 2$ in (10-165), we obtain the ordering of the product basis vectors

$$\begin{aligned} &|x1y1\rangle \ , \quad |x1y2\rangle \ , \quad |x2y1\rangle \ , \quad |x2y2\rangle \ , \\ &|y1x1\rangle \ , \quad |y1x2\rangle \ , \quad |y2x1\rangle \ , \quad |y2x2\rangle \ , \end{aligned} \tag{10-177}$$

where $|xayb\rangle$ represents the vector $|\psi^{(X_1)}_{\mathbf{k}_z a}\psi^{(X_2)}_{\mathbf{k}_y b}\rangle$.

9. The eigenvalues of $M(C_1)$ and $M(C_2)$ are found to be

$$(C_1, C_2) = (0,2) \ , \quad (0,-2) \ , \quad (2i,0) \ , \quad (-2i,0) \ ,$$

and each has the degeneracy 2. By comparison with Table 10.19-1, we get the CG series

$$*X(1) \otimes *X(2) = *X(1) \oplus *X(2) \oplus *X(3) \oplus X(4) \ . \tag{10-178}$$

The eigenvalues of $M(C(s))$ are found to be $\pm 1, \pm i$. Substituting the four sets of eigenvalues of $(C_1, C_2, C(s))$ — $(0,2,1), (0,-2,1), (2i,0,-i)$, and $(-2i,0,-i)$ - into the eigenequation (10-145), we obtain the four eigenvectors listed in the odd rows of Table 10.19-2. They are the CG coefficients for the first component $a'' = 1$.

10. From (10-154) and Table 10.19-1 the second component of the CG coefficients can be expressed as

$$\begin{aligned} U^{(X_j)}_{\mathbf{k}_z 2} &= \frac{M(\{C_{2a}|\tau\}')}{\Delta^{(X_j)}_{21}(C_{2a})} U^{(X_j)}_{\mathbf{k}_z 1} = -M(\{C_{2a}|\tau\}') U^{(X_j)}_{\mathbf{k}_z 1} \ , \quad j = 1,2, \\ U^{(X_j)}_{\mathbf{k}_z 2} &= \frac{M(\{\sigma_{da}|0\})}{\Delta^{(X_j)}_{21}(\sigma_{da})} U^{(X_j)}_{\mathbf{k}_z 1} = i(-1)^j M(\{\sigma_{da}|0\}) U^{(X_j)}_{\mathbf{k}_z 1} \ , \quad j = 3,4 \ . \end{aligned} \tag{10-179}$$

With (10-179) and (10-176c), as well as the odd rows in Table 10.19-2 we can find $U^{(X_j)}_{\mathbf{k}_z 2}$, for example,

$$U^{(X_3)}_{\mathbf{k}_z 2} = \frac{i}{\sqrt{8}} \begin{pmatrix} & & & & & & & 1 \\ & & & & & & 1 & \\ & & & & & 1 & & \\ & & & & 1 & & & \\ & & & 1 & & & & \\ & & 1 & & & & & \\ & 1 & & & & & & \\ 1 & & & & & & & \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ -1 \\ -1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{8}} \begin{pmatrix} i \\ i \\ -i \\ -i \\ -i \\ i \\ -i \\ i \end{pmatrix} \tag{10-180}$$

The CG coefficients $U^{(X_j)}_{\mathbf{k}_z 2}$ are listed in the even rows of Table 10.19-2.

11. To obtain the CG coefficients with $\sigma'' \neq 1$, we in general need to use (10-158). However, for the case where

$$\begin{aligned} &*\mathbf{k} = *\mathbf{k}' = *\mathbf{k}'' , \\ &\{\beta_\sigma|\mathbf{V}_\sigma\} = \{\beta_{\sigma'}|\mathbf{V}_{\sigma'}\} = \{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\} , \end{aligned} \tag{10-181}$$

it is a very simple matter to obtain the CG coefficients with $\sigma'' \neq 1$ from those with $\sigma'' = 1$. For example, in our case here for $\sigma'' = 2, \{\beta_{\sigma''}|\mathbf{V}_{\sigma''}\} = C^+_{31}$,

$$\begin{aligned} \psi^{X(1)}_{\mathbf{k}_z} &= C^+_{31}\psi^{X(1)}_{\mathbf{k}_z} \\ &= \frac{1}{\sqrt{8}}(|y1z1\rangle - i|y1z2\rangle - i|y2z1\rangle + |y2z2\rangle - |z1y1\rangle + i|z1y2\rangle + i|z2y1\rangle + |z2y2\rangle) . \end{aligned}$$

Hence the CG coefficients for $\sigma'' = 2$ and 3 result from a cyclic permutation of x, y, and z in Table 10-19-2.

Similarly, by letting $*\mathbf{k} = \Gamma$, we can get the CG coefficients for $*X(1) \otimes *X(2) \to \Gamma(\nu'')$.

10.19.2. The CG coefficients of O^7_h for $*X(1) \otimes *W(1) \to *\Delta(\nu'')$

We now turn to a more general example for which the three wave vector stars $*\mathbf{k}, *\mathbf{k}'$, and $*\mathbf{k}''$ are all different and the multiplicity may be larger than one.

1. The wave vector selection rule is given in (10-143c), it is

$$*X \otimes *W = 2 * \Delta + *W . \tag{10-182a}$$

2. Pick out $*\mathbf{k}'' = *\Delta$.

3. The canonical wave vectors are chosen to be

$$\begin{matrix} \text{Star } X & \text{Star } W & \text{Star } \Delta \\ \mathbf{k} = (\tfrac{1}{2}, \tfrac{1}{2}, 0) , & \mathbf{k}' = (\tfrac{1}{2}, \tfrac{1}{4}, \tfrac{3}{4}) , & \mathbf{k}'' = (\tfrac{1}{4}, \tfrac{1}{4}, 0) . \end{matrix} \tag{10-182b}$$

4. The coset representatives and $\mathbf{k}_\sigma$ for star X are identical to (10-169) and (10-170) respectively, while the coset representatives $\{\beta_{\sigma'}|\mathbf{V}_{\sigma'}\}$ and $\mathbf{k}'_{\sigma'}$ for star W are listed in Table 10.19-3.

It should be noted that although the wave vector, that is, $\mathbf{k}' = (\frac{1}{2}, -\frac{1}{4}, \frac{1}{4})$, is equivalent to $(\frac{1}{2}, \frac{3}{4}, \frac{1}{4})$, the former is *not replaceable* by the latter; errors will occur if this is done.

5. From

$$\mathbf{k}_2 + \mathbf{k}'_5 = \mathbf{k}'' + (011) , \quad \mathbf{k}_3 + \mathbf{k}'_6 = \mathbf{k}'' + (001) , \tag{10-183}$$

it is seen that the index pairs are $(\tau\tau') = (25)$ and $(\sigma\sigma') = (36)$.

6. The irreps $D^{(X)(\nu)}$ and $D^{(W)(\nu')}$ are given in Tables 10.19-1 and 10.15-5 respectively.

7. Δ is an internal point, hence its representation group $\mathbf{G}'_\Delta$ is isomorphic to the little co-group, the point group C_{4v}. From Table 8.3-6, we know that the CSCO-I of C_{4v} is $C = (2C_{4z}, 2\sigma)$. We choose $C(s) = \sigma_y$; this corresponds to choosing (x, y) as the basis vectors of the two-dimensional irrep of C_{4v}. Due to the isomorphism between $\mathbf{G}'_\Delta$ and C_{4v}, the CSCO-I of $\mathbf{G}'_\Delta$ is

$$C = (C_3, C_4) , \quad C_3 = \{C^+_{4x}|\tau\}' + \{C^-_{4z}|\tau'\} , \quad C_4 = \{\sigma_x|\tau\}' + \{\sigma_y|\tau\}' , \tag{10-184}$$

and the operator $C(s)$ is

$$C(s) = \{\sigma_y|\tau\}' . \tag{10-185}$$

By means of (10-163) and Table 10.19-1 and 10.15-5 we can construct the following submatrices:

$$\left[D^{(*X)(1)}(\{C_{4z}^{+}|\tau\})\right] = \begin{matrix} & 2 & 3 \\ 2 & 0 & \kappa \\ 3 & \lambda & 0 \end{matrix}(-i)\,, \quad \left[D^{(*X)(1)}(\{C_{4z}^{-}|\tau\})\right] = -i\begin{pmatrix} 0 & \lambda \\ \kappa & 0 \end{pmatrix},$$

$$\left[D^{(*X)(1)}(\{\sigma_x|\tau\})\right] = -i\begin{pmatrix} \kappa & 0 \\ 0 & \lambda \end{pmatrix}, \qquad \left[D^{(*X)(1)}(\{\sigma_y|\tau\})\right] = -i\begin{pmatrix} \lambda & ,0 \\ 0, & \kappa \end{pmatrix}, \tag{10-186}$$

$$\left[D^{(*W)(1)}(\{C_{4z}^{+}|\tau\})\right] = \begin{matrix} & 5 & 6 \\ 5 & 0 & -\mu i \\ 6 & \mu^* & 0 \end{matrix} e^{-\pi i/4}\,, \quad \left[D^{(*W)(1)}(\{C_{4z}^{-}|\tau\})\right] = e^{-\pi i/4}\begin{pmatrix} 0 & -\mu^* i \\ \mu & 0 \end{pmatrix},$$

$$\left[D^{(*W)(1)}(\{\sigma_x|\tau\})\right] = e^{-\pi i/4}\begin{pmatrix} \kappa i & 0 \\ 0 & -\kappa \end{pmatrix}, \qquad \left[D^{(*W)(1)}(\{\sigma_y|\tau\})\right] = e^{-\pi i/4}\begin{pmatrix} -\varphi i & 0 \\ 0 & \varphi \end{pmatrix}.$$

The 2×2 matrices $\kappa, \lambda, \ldots,$ are defined in Eq. (10-172).

8. Using (10-164) and (10-186), we obtain

$$M(\{C_{4z}^{+}|\tau\}') = \begin{matrix} & 25 & 36 \\ 25 & & \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\mu \\ 36 & \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}\mu^* & \end{matrix}, M(\{C_{4z}^{-}|\tau\}') = \begin{pmatrix} & \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\mu^* \\ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\mu & \end{pmatrix},$$

$$M(\{\sigma_x|\tau\}') \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\kappa & \\ & \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}\kappa \end{pmatrix}, M(\{\sigma_y|\tau\}') = \begin{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\varphi & \\ & \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\varphi \end{pmatrix}. \tag{10-187}$$

By setting $(\tau\tau') = (25), (\sigma\sigma') = (36)$, and $h_\nu = h_{\nu'} = 2$ in Eq. (10-165), we get the ordering for the eight product basis vectors:

$$\begin{aligned} &|2151\rangle\,, \quad |2152\rangle\,, |2251\rangle\,, \quad |2252\rangle\,, \\ &|3161\rangle\,, \quad |3162\rangle\,, |3261\rangle\,, \quad |3262\rangle\,. \end{aligned} \tag{10-188}$$

9. The eigenvalues of the matrices $M(C_3) = M(\{C_{4z}^{+}|\tau\}') + M(\{C_{4z}^{-}|\tau\}')$ and $M(C_4) = M(\{\sigma_x|\tau\}') + M(\{\sigma_y|\tau\}')$ are found to be

$$\begin{aligned} &\text{Single roots: } (2,2), (2,-2), (-2,2), (-2,-2)\,, \\ &\text{Quartet root: } (0,0)\,, \end{aligned} \tag{10-189}$$

which corresponds, according to Table 8.3-6, to the point group reps A_1, A_2, B_1, B_2, and E, respectively. The first four are one dimensional, and the last one is two dimensional. We use $\Delta(1)$–$\Delta(5)$ to denote the corresponding reps for the group $\mathbf{G}'_\Delta$. The degeneracy 4 divided by the dimensionality 2 gives the number of times that the irrep $\Delta(5)$ occurs in the rep $*X(1) \otimes *W(1)$. Therefore, we have the CG series:

$$*X(1) \otimes *W(1) = *\Delta(1) \oplus *\Delta(2) \oplus *\Delta(3) \oplus *\Delta(4) \oplus 2 * \Delta(5)\,. \tag{10-190}$$

For the first four single roots, we can immediately find the corresponding eigenvectors, as listed in the first four rows of Table 10.19-4. For the quartet root (0, 0), a further diagonalization of the matrix $M(C(s))$ is required. Its eigenvalues $a'' = 1$ and -1 correspond to the first and second components of the rep $\Delta(5)$, respectively. When we substitute the eigenvalues (0, 0, 1) of $(C_3, C_4, C(s))$ into their eigenequations, a degeneracy of 2 remains. Consequently there exist two linearly independent solutions. The two orthogonal eigenvectors can be chosen as

$$\begin{aligned} U^{(\theta=1)}_{\mathbf{k}'',1} &= \frac{1}{2}(1,-1,-1,-1,0,0,0,0)\,, \\ U^{(\theta=2)}_{\mathbf{k}'',1} &= \frac{1}{2}(0,0,0,0,1,i,-1,i)\,. \end{aligned} \tag{10-191}$$

10. It is known that the matrix for the element C_{4z} in the rep E of C_{4v} is

$$D^{(E)}(C^+_{4z}) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\,. \tag{10-192}$$

Hence (10-154) now reads

$$U^{(\theta)}_{\mathbf{k}''2} = \frac{1}{D^{(E)}_{21}(C^+_{4z})} M(\{C^+_{4z}|\tau\}')U^{(\theta)}_{\mathbf{k}''1}\,. \tag{10-193}$$

From (10-187) and (10-191)–(10-193) we can calculate $U^{(\theta)}_{\mathbf{k}''2}$; the result is listed in Table 10.19-4.

11. Using (10-158), we can get the CG coefficients with $\sigma \neq 1$ which are not listed here.

10.20. The Double Space Groups

So far we have only considered the single–valued reps of space groups. We now turn to the double–valued reps of space groups.

Corresponding to the space group $\mathbf{G}$ of (10-19b), we have the double space group $\mathbf{G}^\dagger$,

$$\mathbf{G}^\dagger = \{\{\alpha|\mathbf{V}(\alpha)+\mathbf{R}_n\}:\quad \alpha \in \mathbf{G}^\dagger_0,\quad \mathbf{R}_n \in L\}\,, \tag{10-194}$$

where $\mathbf{G}^\dagger_0$ is the double point group defined by (8-121b). Note that

$$\mathbf{V}(\tilde{\alpha}) = \mathbf{V}(\alpha)\,,\quad \tilde{\alpha}\mathbf{V}(\beta) = \alpha\mathbf{V}(\beta)\,. \tag{10-195}$$

In the vector (single–valued) rep space, the representation of $\mathbf{G}^\dagger$ forms a group which is isomorphic to $\mathbf{G}$. In the spinor (double–valued) rep space, the representation of $\mathbf{G}^\dagger$ forms a rep group, denoted by

$$\mathcal{G}^\dagger = \{\{\alpha|\mathbf{V}(\alpha)+\mathbf{R}_n\}:\alpha \in \mathcal{G}^\dagger_0,\, \mathbf{R}_n \in L\}\,, \tag{10-196}$$

where $\mathcal{G}^\dagger_0$ is the rep group of the double point group $\mathbf{G}^\dagger_0$. Among the elements of the rep group $\mathcal{G}^\dagger$, only half the elements are linearly independent, and they obey the multiplication rule

$$\{\alpha_i|\mathbf{V}(\alpha_i)\}\{\alpha_j|\mathbf{V}(\alpha_j)\} = \theta(i,j)\{\alpha_{ij}|\alpha_i\mathbf{V}(\alpha_j)+\mathbf{V}(\alpha_i)\}\,, \tag{10-197}$$

where the factor system $\theta(i,j)$ is defined by (8-136b), and can be found in Table 10-.21-1 for the group O and its subgroups.

The double little group is

$$\mathbf{G}(\mathbf{k})^\dagger = \{\{\gamma_i|\mathbf{V}(\gamma_i)+\mathbf{R}_n\}:\gamma_i \in \mathbf{G}_0(\mathbf{k})^\dagger,\quad \mathbf{R}_n \in L\}\,. \tag{10-198}$$

In spinor rep space and the eigenspace $\mathcal{L}_\mathbf{k}$ defined by (10-54b), the representation of the double little group form the "double rep group" $\mathcal{G}'_\mathbf{k}$ of order $2m|G_0(\mathbf{k})|$ [compare with Eq. (10-70)],

$$\mathcal{G}'_\mathbf{k} = \{R_i : i = 1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|\}_{2m}\,,$$

Table 10.19-3. The coset representatives $\{\beta_{\sigma'}|\mathbf{V}_{\sigma'}\}$ and $\mathbf{k}'_{\sigma'}$ for the star W.

σ'	1	2	34	5	6	
$\{\beta_{\sigma'}\|\mathbf{V}_{\sigma'}\}$	$\{\epsilon\|0\}$	$\{C_{2y}\|0\}$	$\{C_{31}^{+}\|0\}$	$\{C_{33}^{+}\|0\}$	$\{C_{31}^{-}\|0\}$	$\{C_{32}^{-}\|0\}$
$\mathbf{k}'_{\sigma'}$	$(\frac{1}{2}\frac{1}{4}\frac{3}{4})$	$(\frac{1}{2}-\frac{1}{4}\frac{1}{4})$	$(\frac{3}{4}\frac{1}{2}\frac{1}{4})$	$(\frac{1}{4}\frac{1}{2}-\frac{1}{4})$	$(\frac{1}{4}\frac{3}{4}\frac{1}{2})$	$(-\frac{1}{4}\frac{1}{4}\frac{1}{2})$

Table 10.19-4. The CG coefficients $\left(\begin{array}{c|c} X(1)W(1) & \Delta(\nu'')\theta \\ \sigma a\ \sigma' a' & 1a'' \end{array}\right)$ of O_h^7 for $*X(1)\otimes *W(1)$ and $\sigma''=1$.

						$\sigma a\sigma' a'$							
		(C_3,C_4)	$C(s)$	θ	N	$\|2151\rangle$	$\|2152\rangle$	$\|2251\rangle$	$\|2252\rangle$	$\|3161\rangle$	$\|3162\rangle$	$\|3261\rangle$	$\|3262\rangle$
$\Delta(1)$	A_1	$(2,2)$			$\frac{1}{\sqrt{8}}$	1	-1	1	1	1	$-i$	1	i
$\Delta(2)$	A_2	$(2,-2)$			$\frac{1}{\sqrt{8}}$	1	1	1	-1	-1	$-i$	-1	i
$\Delta(3)$	B_1	$(-2,2)$			$\frac{1}{\sqrt{8}}$	1	-1	1	1	-1	i	-1	$-i$
$\Delta(4)$	B_2	$(-2,-2)$			$\frac{1}{\sqrt{8}}$	1	1	1	-1	1	i	1	$-i$
$\Delta(5)$	E	$(0,0)$	1	1	$\frac{1}{2}$	1	-1	-1	-1				
			-1	1	$\frac{1}{2}$					1	$-i$	-1	$-i$
$\Delta(5)$	E	$(0,0)$	1	2	$\frac{1}{2}$					1	i	-1	i
			-1	2	$\frac{1}{2}$	1	1	-1	1				

$$R_i = \{\gamma_i|\mathbf{V}(\gamma_i)\}' = \exp[i\mathbf{k}\cdot\mathbf{V}(\gamma_i)]\,\{\gamma_i|\mathbf{V}(\gamma_i)\}\ . \tag{10-199}$$

The multiplication relations for the "double rep group" are

$$R_iR_j = \theta(i,j)\eta(i,j)R_{ij}\ , \tag{10-200}$$

where the factor system $\eta(i,j)$ is still given by Eq. (10-67d) or (10-80a).

Equation (10-200) has the same form as (10-67a). Consequently, the problem of finding the double–valued irreps of space groups is also as easy as that of finding irreps of point groups with maximal order equal to 48, while with the conventional method (Bradley 1972), one needs to deal with a group of order $2m|\mathbf{G}_0(\mathbf{k})|$, which can be as high as $2\times 4\times 48 = 384$. Therefore, the rep group approach to the double–valued reps of space groups drastically simplifies the problem.

The procedure for constructing the full double–valued rep matrices $D^{(*\mathbf{k})(\nu)}$ of a space group is the same as that for the single–valued rep matrices with the following modifications: In constructing the matrices $\mathcal{D}(\{\alpha|\mathbf{a}\})$ of (10-118), the product $\beta_\tau^{-1}\alpha\beta_\sigma$ should be calculated with the *double point group multiplication rule*, and the $(\tau\sigma)$ block in (10-118) is again equal to $\Delta(\gamma)$ if $\beta_\tau^{-1}\alpha\beta_\sigma = \gamma$ belongs to the *double point group* $\mathbf{G}_0(\mathbf{k})^\dagger$, and $\Delta(-\gamma) = -\Delta(\gamma)$.

The technique for computing the CG coefficients for the double space group follows the discussion of Sec. 10.18. The only point worth mentioning is that the product of two spinor reps is a vector rep, while the product of a spinor rep and a vector rep is a spinor rep.

Example: Find the double–valued irreps of D_{4h}^{14} at the point Y. The group elements of D_{4h}^{14} are given in Sec. 10.6. The wave vector for the point Y and its symmetric group can be found from Table 3.6 in Bradley (1972, p. 116): $\mathbf{k}_y = (\alpha\frac{1}{2}0)$, and $\mathbf{G}_0(Y) = \mathcal{C}_{2v} = (\varepsilon, C_{2x}, \sigma_y, \sigma_z)$.

The group table for the rep group $\mathcal{G}_Y'$ with the factor system $\eta(i,j)$ is given in Table 10.20-1 [where $\mathbf{v} = (\frac{1}{2}\frac{1}{2}\frac{1}{2})$]. For the double point group $\mathcal{C}_{2v}^\dagger$, the group table can be found from Table 10.21-1, and is given in Table 10.20-2. Combining Tables 10.20-1 and 10.20-2, we obtain the group table for the "double rep group" $\mathcal{G}_Y^\dagger$, shown in Table 10.20-3. Choosing $C(s) = R_2$, we can easily find the double-valued irreps $\Delta^{(Y)}$ of D_{4h}^{14}, listed in Table 10.20-3.

Table 10.20-1. Group table of G_Y'.

$\{\varepsilon\|\ 0\}$	$\{C_{2x}\|\mathbf{v}\}'$	$\{\sigma_y\|\mathbf{v}\}'$	$\{\sigma_z\|\ 0\}$
1	2	3	4
2	−1	−4	3
3	−4	−1	2
4	3	2	1

Table 10.20-2. Group table of $C_{2v}^\dagger$.

ε	C_{2x}	σ_y	σ_z
1	2	3	4
2	−1	4	−3
3	−4	−1	2
4	3	−2	−1

Table 10.20-3. Group table of $G_Y^{\prime\dagger}$ and double–valued rep of D_{4h}^{14}.

	R_1	R_2	R_3	R_4
	1	2	3	4
	2	1	−4	−3
	3	4	1	2
	4	3	−2	−1
$\Delta^{(Y)}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$

Based on the rep group approach, a program (Ping 1989) and its upgraded version (Chen & Ping 1999) have been written with the following functions

1. Computing the subgroup–symmetry adapted single–valued and double–valued irreps of space groups. The subgroup can be chosen either according to one's requirements or by the computer.

2. Computing the wave vector selection rules, the CG series and subgroup–symmetry adapted CG coefficients of space groups for Kronecker products of any two reps, that is, vector ⊗ vector, vector ⊗ spinor and spinor ⊗ spinor.

Ex. 10.1. From the generators of D_{4h}^{19}, $\{C_{4z}|0\frac{1}{2}0\}$, $\{C_{2x}|000\}$, $\{I|000\}$, find the remaining group elements.

Ex. 10.2. Find the single–valued and double–valued irreps of D_{4h}^{14} at the point T, $\mathbf{p} = (\alpha, \frac{1}{2}\frac{1}{2})$, $\mathbf{G}_0(T) = (\varepsilon, C_{2x}, \sigma_y, \sigma_z)$. The group table of D_{4h} is given in Table 10.20-4.

Table 10.20-4. Group table for D_{4h}.

e	C_{2x}	C_{2y}	C_{2z}	C_{4z}^{-}	C_{4z}^{+}	C_{2a}	C_{2b}
1	2	3	4	5	6	7	8
2	1	4	3	7	8	5	6
3	4	1	2	8	7	6	5
4	3	2	1	6	5	8	7
5	8	7	6	4	1	2	3
6	7	8	5	1	4	3	2
7	6	5	8	3	2	1	4
8	5	6	7	2	3	4	1

Ex. 10.3. Find the irreducible bases for the single–valued irreps of D_{4h}^{14} at the point T.

Ex. 10.4. Find the single–valued and double–valued irreps of D_{4h}^{14} at the point $X, \mathbf{p} = (0, \frac{1}{2}, 0)$, $\mathbf{G}_0(X) = D_{2h} = (e, C_{2x}, C_{2y}, C_{2z}, I, \sigma_x, \sigma_y, \sigma_z)$.

Ex. 10.5. Find the single–valued and double–valued irreps of D_{4h}^{19} at the points $U[\mathbf{p} = (\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}+\alpha)]$ and $Y[\mathbf{p} = (-\alpha, \alpha, \frac{1}{2})]$. $\mathbf{G}_0(U) = \mathcal{C}_{2v} = (e, C_{2a}, \sigma_z, \sigma_{db})$, $\mathbf{G}_0(Y) = \mathcal{C}_{2v} = (e, C_{2b}, \sigma_z, \sigma_{da})$. [The space group D_{4h}^{19} belongs to the tetragonal crystal system with body–centered Bravais lattice Γ_q^v. The operations of the group elements of D_{4h} on the primitive translations $\mathbf{t}_i$ can be read out from Table 10.21-2 under the heading Γ_c^v (the body-centered cubic).]

Ex. 10.6. Find the double–valued irreps for the little group of O_h^7 at the point W.

10.21. Appendix

Table 10.21-1. The group table of $O^{\dagger}$

E	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
C_{2x}	2	$\tilde{1}$	4	$\tilde{3}$	$\tilde{8}$	7	$\tilde{6}$	5	10	$\tilde{9}$	12	$\tilde{11}$	$\tilde{16}$	21	$\tilde{20}$	13	$\tilde{23}$	19	$\tilde{18}$	15	$\tilde{14}$	24	17	$\tilde{22}$
C_{2y}	3	$\tilde{4}$	$\tilde{1}$	2	$\tilde{6}$	5	8	$\tilde{7}$	11	$\tilde{12}$	$\tilde{9}$	10	$\tilde{24}$	$\tilde{17}$	19	22	14	20	$\tilde{15}$	$\tilde{18}$	$\tilde{23}$	$\tilde{16}$	21	13
C_{2z}	4	3	$\tilde{2}$	$\tilde{1}$	$\tilde{7}$	$\tilde{8}$	5	6	12	11	$\tilde{10}$	$\tilde{9}$	22	23	$\tilde{18}$	24	21	15	20	$\tilde{19}$	$\tilde{17}$	$\tilde{13}$	$\tilde{14}$	$\tilde{16}$
C_{31}^{+}	5	$\tilde{6}$	$\tilde{7}$	$\tilde{8}$	$\tilde{9}$	12	10	11	1	3	4	2	19	22	21	15	13	14	$\tilde{17}$	23	$\tilde{16}$	$\tilde{18}$	24	$\tilde{20}$
C_{32}^{+}	6	5	8	$\tilde{7}$	11	$\tilde{10}$	12	9	$\tilde{3}$	1	$\tilde{2}$	4	15	16	23	$\tilde{19}$	24	17	14	$\tilde{21}$	22	20	$\tilde{13}$	$\tilde{18}$
C_{33}^{+}	7	$\tilde{8}$	5	6	12	9	$\tilde{11}$	10	$\tilde{4}$	2	1	$\tilde{3}$	$\tilde{20}$	13	17	18	$\tilde{22}$	$\tilde{23}$	21	14	24	15	16	$\tilde{19}$
C_{34}^{+}	8	7	$\tilde{6}$	5	10	11	9	$\tilde{12}$	$\tilde{2}$	$\tilde{4}$	3	1	18	$\tilde{24}$	14	20	16	$\tilde{21}$	$\tilde{23}$	$\tilde{17}$	13	19	22	15
C_{31}^{-}	9	12	10	11	1	$\tilde{2}$	$\tilde{3}$	$\tilde{4}$	$\tilde{5}$	7	8	6	17	18	16	$\tilde{21}$	$\tilde{19}$	$\tilde{22}$	13	$\tilde{24}$	15	14	20	23
C_{32}^{-}	10	$\tilde{11}$	$\tilde{9}$	12	2	1	$\tilde{4}$	3	8	$\tilde{6}$	5	7	$\tilde{23}$	19	13	14	18	$\tilde{24}$	$\tilde{16}$	22	$\tilde{20}$	21	15	17
C_{33}^{-}	11	10	$\tilde{12}$	$\tilde{9}$	3	4	1	$\tilde{2}$	6	8	$\tilde{7}$	5	14	20	22	23	15	16	$\tilde{24}$	$\tilde{13}$	19	$\tilde{17}$	$\tilde{18}$	21
C_{34}^{-}	12	$\tilde{9}$	11	$\tilde{10}$	4	$\tilde{3}$	2	1	7	5	6	$\tilde{8}$	21	15	24	17	$\tilde{20}$	13	22	16	$\tilde{18}$	23	$\tilde{19}$	$\tilde{14}$
C_{4x}^{+}	13	$\tilde{16}$	22	24	21	17	$\tilde{23}$	14	18	19	15	$\tilde{20}$	2	5	12	1	7	10	$\tilde{9}$	11	$\tilde{8}$	4	6	$\tilde{3}$
C_{4y}^{+}	14	$\tilde{23}$	$\tilde{17}$	21	19	15	18	20	16	$\tilde{24}$	22	13	10	3	5	11	1	8	$\tilde{6}$	$\tilde{7}$	2	$\tilde{9}$	4	12
C_{4z}^{+}	15	19	20	$\tilde{18}$	22	24	13	16	17	14	23	21	5	11	4	6	12	1	3	$\tilde{2}$	$\tilde{9}$	$\tilde{7}$	$\tilde{10}$	$\tilde{8}$
C_{4x}^{-}	16	13	$\tilde{24}$	22	14	23	17	$\tilde{21}$	$\tilde{19}$	18	20	15	1	8	11	$\tilde{2}$	6	9	10	$\tilde{12}$	5	3	$\tilde{7}$	4
C_{4y}^{-}	17	21	14	23	15	$\tilde{19}$	$\tilde{20}$	18	$\tilde{22}$	13	16	24	12	1	6	9	$\tilde{3}$	7	5	8	4	11	$\tilde{2}$	$\tilde{10}$
C_{4z}^{-}	18	$\tilde{20}$	19	15	13	16	$\tilde{22}$	$\tilde{24}$	$\tilde{21}$	$\tilde{23}$	14	17	7	10	1	8	9	$\tilde{4}$	2	3	12	5	11	6
C_{2a}	19	$\tilde{15}$	$\tilde{18}$	$\tilde{20}$	$\tilde{16}$	13	$\tilde{24}$	22	14	$\tilde{17}$	21	$\tilde{23}$	$\tilde{6}$	$\tilde{9}$	2	5	10	3	$\tilde{1}$	4	$\tilde{11}$	$\tilde{8}$	12	7
C_{2b}	20	18	$\tilde{15}$	19	$\tilde{24}$	22	16	$\tilde{13}$	23	$\tilde{21}$	$\tilde{17}$	14	8	$\tilde{12}$	3	$\tilde{7}$	11	$\tilde{2}$	$\tilde{4}$	$\tilde{1}$	10	$\tilde{6}$	$\tilde{9}$	5
C_{2c}	21	$\tilde{17}$	23	$\tilde{14}$	$\tilde{18}$	$\tilde{20}$	19	15	13	22	24	$\tilde{16}$	$\tilde{9}$	4	$\tilde{8}$	12	2	5	$\tilde{7}$	6	$\tilde{1}$	$\tilde{10}$	$\tilde{3}$	$\tilde{11}$
C_{2d}	22	$\tilde{24}$	$\tilde{13}$	$\tilde{16}$	$\tilde{17}$	21	14	23	15	20	$\tilde{18}$	19	3	$\tilde{7}$	$\tilde{9}$	4	5	11	$\tilde{12}$	$\tilde{10}$	$\tilde{6}$	$\tilde{1}$	$\tilde{8}$	2
C_{2e}	23	14	$\tilde{21}$	$\tilde{17}$	20	$\tilde{18}$	15	$\tilde{19}$	24	16	$\tilde{13}$	22	11	$\tilde{2}$	$\tilde{7}$	$\tilde{10}$	4	6	8	$\tilde{5}$	3	$\tilde{12}$	$\tilde{1}$	$\tilde{9}$
C_{2f}	24	22	16	$\tilde{13}$	23	$\tilde{14}$	21	17	$\tilde{20}$	15	$\tilde{19}$	$\tilde{18}$	4	6	$\tilde{10}$	$\tilde{3}$	$\tilde{8}$	12	11	9	$\tilde{7}$	$\tilde{2}$	$\tilde{5}$	$\tilde{1}$

Table 10.21-2. The operations of the point group elements on the primitive translation $\mathbf{t}_i$. Note, that here we use i in place of $\mathbf{t}_i$. For example: for Γ_c^f, $C_{2x}\ \mathbf{t}_2 = -\mathbf{t}_1 + \mathbf{t}_3$, $C_{31}^+\ \mathbf{t}_1 = \mathbf{t}_2$.

	simple cubic (Γ_c)			face-centered cubic (Γ_c^f)			body-centered cubic (Γ_c^v) body-centered tetragonal (Γ_g^v)		
ϵ	1	2	3	1	2	3	1	2	3
C_{2x}	1	−2	−3	−1	−1+3	−1+2	−1−2−3	3	2
C_{2y}	−1	2	−3	−2+3	−2	1−2	3	−1−2−3	1
C_{2z}	−1	−2	3	2−3	1−3	−3	2	1	−1−2−3
C_{31}^+	2	3	1	2	3	1	2	3	1
C_{32}^+	2	−3	−1	−2	1−2	−2+3	−1−2−3	1	3
C_{33}^+	−2	3	−1	1−3	−3	2−3	1	−1−2−3	2
C_{34}^+	−2	−3	1	−1+3	−1+2	−1	3	2	−1−2−3
C_{31}^-	3	1	2	3	1	2	3	1	2
C_{32}^-	−3	1	−2	−1+2	−1	−1+3	2	−1−2−3	3
C_{33}^-	−3	−1	2	1−2	−2+3	−2	1	3	−1−2−3
C_{34}^-	3	−1	−2	−3	2−3	1−3	−1−2−3	2	1
C_{4x}^+	1	2	−2	2−3	−1+2	2	−3	−1	1+2+3
C_{4y}^+	−3	2	1	3	−1+3	−2+3	1+2+3	−1	−2
C_{4z}^+	2	−1	3	1−3	1	1−2	−3	1+2+3	−2
C_{4x}^-	1	−3	2	−2+3	3	−1+3	−2	1+2+3	−1
C_{4y}^-	3	2	−1	1−2	1−3	1	−2	−3	1+2+3
C_{4z}^-	−2	1	3	2	2−3	−1+2	1+2+3	−3	−1
C_{2a}	2	1	−3	−1+2	−2+3	3	−1	−2	1+2+3
C_{2b}	−2	−1	−3	−2	−1	−3	−2	−1	−3
C_{2c}	3	−2	1	−1+2	2	2−3	−1	1+2+3	−3
C_{2d}	−1	3	2	1	1−2	1−3	1+2+3	−2	−3
C_{2e}	−3	−2	−1	−3	−2	−1	−3	−2	−1
C_{2f}	−1	−3	−2	−1	−3	−2	−1	−3	−2

Appendix

Table A1. Dimensions of irreps of the permutation groups S_f ($f \leq 6$)and unitary groups SU_n ($n \leq 6$).

	[1]	[2]	[11]	[3]	[21]	[1^3]	[4]	[31]	[22]	[211]	[1^4]	[5]	[41]	[32]	[311]	[221]	[21^3]	[1^5]
S_f	1	1	1	1	2	1	1	3	2	3	1	1	4	5	6	5	4	1
SU_3	3	6	3	10	8	1	15	15	6	3	*	21	24	15	6	3	*	*
SU_4	4	10	6	20	20	4	35	45	20	15	1	56	84	60	36	20	4	*
SU_5	5	15	10	35	40	10	70	105	50	45	5	126	224	175	126	75	24	1
SU_6	6	21	15	56	70	20	126	210	105	105	15	252	504	420	336	210	84	6

	[6]	[51]	[42]	[411]	[33]	[321]	[31^3]	[2^3]	[$2^2 1^2$]	[21^4]	[1^6]
S_f	1	5	9	10	5	16	10	5	9	5	1
SU_3	28	35	27	10	10	8	*	1	*	*	*
SU_4	84	140	126	70	50	64	10	10	6	*	*
SU_5	210	420	420	280	175	280	70	50	45	57	*
SU_6	462	1050	1134	840	490	896	280	175	189	35	1

Note that the dim of SU_3 irreps is: $\frac{1}{2}(\lambda+1)(\mu+1)(\lambda+\mu+2)$

Table A2. Phase factors $\epsilon_1(\nu_1\nu_2\nu)$ for the permutation group IDC and SU_n CG coefficients [see Eqs. (4-153) and (7-101)].

$[\nu_1]$	[1]		[2]		[11]		[3]		[1^3]	
$[\nu_2]$	[1]		[1]		[1]		[1]		[1]	
$[\nu]$	[2]	[11]	[3]	[21]	[1^3]	[21]	[4]	[31]	[1^4]	[211]
ϵ_1	1	−1	1	−1	1	1	1	−1	−1	1

$[\nu_1]$	[2]			[11]			[2]		[21]		
$[\nu_2]$	[2]			[11]			[11]		[1]		
$[\nu]$	[4]	[31]	[22]	[1^4]	[211]	[22]	[31]	[211]	[31]	[211]	[22]
ϵ_1	1	−1	1	1	−1	1	1	1	1	1	−1

$[\nu_1]$	[4]		[1^4]		[31]			[211]		
$[\nu_2]$	[1]		[1]		[1]			[1]		
$[\nu]$	[5]	[41]	[21^3]	[1^5]	[41]	[32]	[311]	[311]	[221]	[21^3]
ϵ_1	1	−1	1	1	1	−1	1	1	−1	−1

$[\nu_1]$	[22]		[3]			[1^3]			[3]	
$[\nu_2]$	[1]		[2]			[11]			[11]	
$[\nu]$	[32]	[221]	[5]	[41]	[32]	[221]	[21^3]	[1^5]	[41]	[311]
ϵ_1	1	1	1	−1	1	1	1	1	1	1

$[\nu_1]$	[1^3]		[21]				[21]			
$[\nu_2]$	[2]		[2]				[11]			
$[\nu]$	[311]	[21^3]	[41]	[32]	[311]	[221]	[32]	[311]	[221]	[21^3]
ϵ_1	1	−1	1	−1	1	−1	1	−1	−1	1

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