

Lectures on LQG/LQC

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A School on Loop Quantum Gravity was held at the IMSc during Sept 8 – 18, 2009. In the first week a basic introduction to LQG was provided while in the second week the focus was on the two main application, to cosmology (LQC) and to the black hole entropy. These notes are an expanded written account of the lectures that I gave. These are primarily meant for beginning researchers.

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Preface

It has been felt for a while that our graduate students do not get an opportunity to get an exposure to the non-perturbative, background independent quantum theory of gravity at a pedagogic level. Although there are several excellent reviews and lecture notes available, an opportunity for complementing lectures by discussions is always an added bonus for the students. With this in mind and taking into account of the background preparation of the students, the *School on Loop Quantum Gravity* was organized at IMSc, for a period of 10 days. The first 5 days were devoted to the basics of connection formulation and loop quantization up to sketching steps involved in the quantization of the Hamiltonian constraint. The next 5 days were devoted to the applications to quantum cosmology and to the black hole entropy. In all 20 lectures and 10 tutorials were planned, however some tutorials ‘became’ additional lectures.

These notes are an expanded version of the topics that I covered. In particular the material of chapter 2, sections 4.2.1, 4.2.2, 4.2.3 and appendices 5.1, 5.3, 5.4 have been added. Email discussions on the sections of chapter 4 and appendix 5.4 with Abhay Ashtekar, Martin Bojowald and Madhavan Varadarajan have been very helpful and are gratefully acknowledged. There could still be some differences in the perceptions and formulations, what I have presented is my understanding of the issues.

The other main lecturers at the school were: Prof Amit Ghosh, Saha Institute of Nuclear Physics, Kolkata; Dr Alok Laddha, Raman Research Institute, Bengaluru; Parthasarathi Majumdar, SINP, Kolkata. In addition, Prof Romesh Kaul, IMSc, Dr Kinjal Banerjee, IUCAA, Pune and Ayan Chatterjee, SINP, Kolkata also gave a few lectures. Amit and Alok discussed the connection formulation and loop quantization up to the basic steps in the quantization of the Hamiltonian constraint. Partha, Amit and Ayan discussed classical formulation of isolated horizons and entropy associated with them. Romesh discussed the possibility of a ‘vacuum structure for gravity’ and Alok also briefly discussed the Brown-Kuchar dust model. It is a pleasure to acknowledge their contributions. At least some notes of the topics covered by these will be available in not-too-distant a future.

The funding for the school was provided by the Institute of Mathematical Sciences under the XIth Plan Project entitled *Numerical Quantum Gravity and Cosmology*. It is envisaged that a more specialized workshop at an advanced level will be held in the summer of 2010 with the possibility of a similar School being repeated one more time.

Chapter 1

General Remarks:

1.1 Why a Quantum Theory of Gravity?

This is not a rhetorical question but it is intended to *identify physical context* in which the classical theory of gravity, specifically the Einstein Theory of Gravity also referred to as General Relativity, is *inadequate* and calls for an extension. One has met with inadequacies of classical theories many times and has seen how their quantum versions have alleviated the inadequacies. For example, the classical theory of charges and electromagnetic fields was quite adequate until the hydrogen atom was found to have a central nucleus with an electron going around it. Classical theory predicts that since the electron is necessarily accelerated, it must radiate away its energy and spiral into the proton. Indeed in about 10^{-9} seconds (!) the classical trajectory of a (bound) electron would ‘end’ in the proton. We all know that this is physically wrong and the atoms are known to be stable for billions of years. We also know that the ‘fault’ lies not with the ‘Coulomb law’ (which does get modified) but with the classical *framework* of using well defined trajectories to describe the dynamical evolution for both the electron and the electromagnetic field. Inadequacies of classical theories are also revealed in the black body spectrum, specific heat of solids at low temperatures etc etc and the appropriate quantum theory of matter and electromagnetism cures these problems i.e. gives results consistent with experimental observations. The quantum nature of other interactions such as the strong and the weak is also verified in nuclear and particle physics. What about the gravitational interactions?

Gravitationally bound ‘atoms’ can also be considered. If gravity is described in the Newtonian manner, there is no gravitational radiation from an accelerated motion and the inward spiralling problem will not arise. But Einstein’s theory of gravity is very different and accelerated sources do radiate away energy and the stability issue re-surfaces. Of course the ‘weakness’ of gravitational interaction does not threaten the existence of such gravitationally bound atoms if the decay time is larger than the age of the universe, but in principle possibility exists. In fact Einstein did suggest a need for a quantum theory of gravity [1] almost immediately after GR was constructed¹.

General relativity however uncovered two distinct contexts in which the theory calls for an

¹At that time, the universe was supposed to be eternal and hence, however small the gravitational instability, existence of stable atoms would threaten GR unless gravitational radiation is also terminated at certain stage.

extension – the context of (i) cosmological and black hole singularities and (ii) entropy of black hole horizons. Let us take a little closer look at these contexts.

The cosmological context: Under the assumption of *homogeneity and isotropy*, the space-time metric is described in terms of a single dynamical variable – the scale factor. As long as the energy density is positive and the pressure is not too negative (which is true for the properties of known matter), in an expanding universe (an observational fact), the scale factor vanishes at a finite time in the past. The universe has ‘beginning’, a finite age and the space-time curvature (or gravity) is infinitely large. Thus, a homogeneous, isotropic universe has *singular beginning*. If one relaxes isotropy but retains homogeneity, one has several *types* of space-times. There are now a maximum of *six* dynamical variables. The simplest of these, the vacuum Bianchi I space-time, has three ‘scale factors’ whose time dependence is given by the (exact) Kasner solution. This is also singular. As one evolves back in time, two of the scale factors vanish while the third one diverges. The most complex of these models, the vacuum Bianchi IX space, is also singular and the backward evolution has an *oscillatory* behaviour. Like the Kasner solution, two scale factors begin decreasing and the third one increasing. But after a while, the three scale factors change their behaviour and a different pair begins decreasing. This continues ad infinitum. If the *non-diagonal* metric components are included, then the directions along which contraction/expansion takes place are also ‘rotated’. If one relaxes homogeneity as well, then a beautiful analysis done by Belinskii-Khalatnikov-Lifschitz (BKL), shows that there exists a *general solution* of the vacuum Einstein equations which can be described as smaller and smaller portions of the spatial slice behaving as a homogeneous, Bianchi IX solution. The BKL analysis in particular shows that singular solutions found in the simpler situations are *not* due to high degree of symmetry (homogeneity and isotropy), but even without such symmetries, there exist general solutions which are singular (diverging curvatures) and the nature of singularities can be extremely complicated.

During the sixties Geroch-Penrose-Hawking used another approach to establish the *Singularity theorems* identifying conditions under which singularities are inevitable consequence of classical GR. For these theorems, singular space-times were defined as those *in-extendible space-times which admit at least one causal (time-like or null) geodesic which is incomplete*. Here incompleteness means that the geodesic cannot be defined for all real values of an affine parameter. There are three types of inputs in these theorems: (a) One restricts to a class of space-times which are *causally well-behaved* eg are free from closed causal curves. The space-times which are free of all causal pathologies and are fully deterministic are the so-called *globally hyperbolic* space-times. (b) The space-times are solutions of Einstein equation with the matter stress tensor satisfying suitable *energy condition(s)*. This incorporates that idea that gravity is attractive (for positive mass/energy). These two types of conditions are general requirements for a space-time model to be physically relevant. (c) the third input is a condition that distinguishes specific physical context such as an everywhere *expanding universe* or a gravitational collapse which has proceeded far enough to develop *trapped surfaces*. The presence of the last condition(s) shows that not every solution satisfying the first two conditions is singular (e.g. the Minkowski space-time). Thus, singularity theorems do *not* imply that gravitational interactions *always* produce singularities – the (c) type condition is necessary. While inclusion of (c) will imply singular space-times, it is *not* automatic that this condition is *realized* in the physical world. In our physical world however universe is expanding and it is widely believed that black holes also exist and hence condition (c) *is* realized in nature. Thus, physical contexts exist wherein classical GR is inadequate.

Remark 1: The global hyperbolicity condition implies that the space-time is *stably causal* i.e.

a global time function exists such that each hyper-surface of constant ‘time’ is space-like. Furthermore, a time function can be chosen such that the space-like hypersurfaces are *Cauchy* surfaces. The topology of such space-times is necessarily $\mathbb{R} \times \Sigma$. A Hamiltonian formulation makes sense only in such space-times. Thus, *not every solution* of Einstein equation yields a physically acceptable space-time (i.e. causally well behaved or globally hyperbolic). A Hamiltonian evolution however constructs such space-times ².

Remark 2: In specific solutions, one encounters singularities (regions of diverging curvatures) which are *space-like* (positive mass Schwarzschild solution, homogeneous cosmologies), *time-like* (negative mass Schwarzschild solution) or even *null* (some of the Weyl class of solutions). Singularities that *arise* in an evolution from *non-singular* initial conditions are the ones which strongly display inadequacy of the theory. Typically, these are the space-like singularities. Since the Hamiltonian formulation is an initial value formulation, it can “see” only such singularities.

The Black hole context: Black holes are objects whose ‘interiors’ are inaccessible to far away observers. More precisely, these are space-time geometries that have a *horizon* which leave some regions out of bounds for asymptotic observers. The special class of *stationary* black holes are characterized by a few parameters – mass (M), angular momentum (J) and electric charge (say) (Q). Associated with their horizons are some characteristic parameters – area of the horizon (A), surface gravity at the horizon (κ), angular velocity at the horizon (Ω) and electromagnetic potential at the horizon (Φ). In the seventies, a remarkable set of “laws” governing processes involving black holes were discovered. If in a process a black hole is disturbed (by accreting mass, say) and returns to a stationary state again, then the changes in the parameters obey:

$$\delta M = \frac{\kappa}{8\pi} \delta A + \Omega_H \delta J + \Phi_H \delta Q \quad , \quad \delta A \geq 0 \quad . \quad (1.1)$$

These are very temptingly analogous to the laws of thermodynamics! Especially after one also proves that κ is constant over the surface of the horizon. Bekenstein in fact suggested that area of the horizon be identified with the entropy of a thermodynamic system. This suggests that the surface gravity be identified with a temperature. Hawking subsequently showed that when possibilities of quantum instabilities are taken into account, a black hole can be thought of a black body with temperature $T = \frac{\kappa \ell_P^2}{2\pi}$ and hence $S = \frac{1}{4} \frac{A}{\ell_P^2}$, $\ell_P^2 := G\hbar$. For all other systems we know that thermodynamics is a manifestation of an underlying statistical mechanics of a large number of *microscopic* degrees of freedom. What are these micro-constituents of the black holes? Notice that from far away, only the exterior of a horizon is accessible and so also parameters such as mass and angular momentum. All detailed memory of what collapsed to form the black hole is lost. So these micro-constituents must be distinct from the matter degrees of freedom. They must represent “atoms” of *geometry*. But classical geometry is continuous so how does a particulate nature arise? Perhaps, not just the specific dynamics given by Einstein equation is inadequate but the *framework of classical geometry* itself is inadequate. Note that black hole horizons are *not* regions of high curvatures and geodesic incompleteness occurs in their interiors. Thus, black hole thermodynamics is a *qualitatively different situation*.

In summary, classical GR contains within its domain, physically realizable physical context where the theory is inadequate. At least one of its context involves *highly dynamical* ge-

²One could *analytically extend* such maximally Cauchy evolved solutions further. These will have Cauchy Horizons, an example being Reissner-Nordstrom space-time.

ometries with high curvatures, matter densities etc. Because of these features, it is hard to imagine how any *perturbative approach* can be developed in these contexts. Since gravity (or space-time geometry) is dynamical and a perturbative approach is unlikely to be suitable, it is necessary to have a quantum theory of gravity which *does not use* any fixed background space-time in its *construction*.

1.2 An Essential Feature of Classical Gravity

Let us recall briefly that special relativity combines Newtonian notions of space and time into a single entity, the *space-time* (Minkowski space-time). The analysis of the geometry inferred in a rotating frame indicates that the geometry is non-Euclidean. Principle of equivalence, which identifies uniform acceleration with uniform gravity (in the Newtonian sense), then implies that gravity affects the space-time geometry and since matter affects gravity, it also affects geometry. In the final formulation of the relativistic theory of gravity, the space-time geometry, described by a metric tensor, is a dynamical (changeable) entity with the Newtonian gravity being a manifestation of the curvature. The law governing the matter-geometry interaction is encoded in the Einstein equation. That all observers are on equal footing to formulate the laws of physics implies that all quantities (and equations) be tensor fields (and equations) with respect to *general coordinate transformations*. Note that a general coordinate transformation corresponds to a *change of chart* in the framework of differentiable manifolds.

Such coordinate transformations however have another interpretation in terms of mapping of the manifold (or local regions thereof) into itself – the *active diffeomorphisms*. Under the action of such mappings, the pull-backs and push-forwards, generate “new” tensor fields from the old ones. That is, in a given neighbourhood, we will have the original tensor field and the one obtained via pull-back/push-forward. If $x \rightarrow y(x)$ represents the mapping in terms of local coordinates, then the pulled-back (pushed-forward) quantities are related to the original ones in precisely the same manner as general coordinate transformation³. If the dynamical equations are covariant with respect to general coordinate transformations (coordinate transform of a solution is also a solution), they must also be covariant with respect to the active diffeomorphisms i.e. a configuration and its transform under active diffeomorphism are both solutions if any one of them is. This has far reaching implications.

The Einstein Hole Argument: The active diffeos can be chosen such that they map non-trivially only in some region (‘sub-manifold’) of the manifold. Choose a region which is free of any matter. Assume that the equations determining gravitational field and matter distribution are also tensor equations (i.e. generally covariant). Consider a solution which has certain curvature distribution inside our chosen ‘hole’. Make a diffeo which is non-trivial only inside the hole and change the curvature distribution. This will also be a solution by covariance. Thus we get a situation that even though matter distribution is unchanged, in a region where there is no matter, we can have two ‘different’ gravitational fields i.e. matter

³Let $\phi : p \rightarrow \phi(p)$ be a smooth map of a manifold onto itself. Given a function $f' : M \rightarrow \mathbb{R}$, define another function $f : M \rightarrow \mathbb{R}$ as: $f(p) := f'(\phi(p))$. This function is the *pull-back* of f' and is also denoted as $f := \phi^*(f')$. Likewise, given a vector field X on M define a new vector field X' as: $X'(f')|_{\phi(p)} := X(f)|_p$. The new vector field is called the *push-forward* of X and is also denoted as: $X' = \phi_*(X)$. Now introduce local coordinates x^i around p and y^i around $\phi(p)$. It is easy to see that the components of tensors relative to these coordinates are related in exactly the same manner as though $x \rightarrow y(x)$ is a change of chart.

distribution does *not* determine the gravitational field. But in the non-relativistic limit Newtonian gravity is determined by matter. So *either* the equations should *not* be covariant *or in the absence of any matter available for ‘marking’ points of a manifold, the ‘different’ distributions of curvature must be regarded as describing the ‘same’ gravitational field.* It is the latter possibility that remains once the *covariance of the equations* is accepted. This in turn implies that *it is the equivalence classes of solutions, with respect to the space-time diffeomorphisms, that correspond to physical reality.*

Note: The size of the hole in the hole argument is unimportant. Also, the metric description itself does *not* play a role; one could repeat the argument for any other field. All that is used is that the fields are tensors under general coordinate transformations (chart change), field equations are covariant and the fields are inhomogeneous within a hole. Values of individual fields at any, manifold point are irrelevant but values of fields at points *specified by other fields* are invariant and thus physical.

Since ‘points’, not marked by any *dynamical entity*, have no physical meaning, the only, physically meaningful, questions are of relational nature. That is, it is physically meaningless to ask what is the curvature (or say electric field) “here and now”. The meaningful questions is what is the curvature where a certain field has a certain value. If we had *any* particular field to be fixed (non-dynamical), then with reference to that field we could ask the ‘here and now’ question. Such a field, constitutes a background. Note that the usual non-gravitational theories or in the perturbative treatment of gravity, the space-time geometry (metric) plays the role of a background. Since in the general relativistic theory *all fields including the metric* are fundamentally dynamical, such a theory is *necessarily background free*. The twin features of the framework namely *all fields* on a manifold being dynamical and the fundamental equation being *generally covariant and deterministic*, implies covariance with respect to active diffeomorphisms and physical characterization being in terms of 4-diffeo equivalence classes of fields ⁴.

This is an essential feature of general relativity, much more fundamental than the particular Einstein equations themselves. The challenge is to construct a quantum theory which faithfully incorporates this feature i.e. a quantum theory of gravity must be background free (or at least recover background independence in the classical limit).

This also poses challenges, because we have to construct observables which are space-time diffeomorphism invariant. These alone could characterise specific equivalence classes of space-times and this problem is not understood even classically for spatially compact case and in absence of matter! Note that curvature invariants, although scalars, are local and *not* diffeo invariants. Hence these cannot be physical observables. Consequently identifying a physical state corresponding to (say) Minkowski space-time is much harder.

For a more detailed discussion of these conceptual issues, see [2].

⁴Since we have taken (differential) equations as specifying a presentation of a theory, the manifold *cannot* be thought of as a background, but rather part of the specification of the theory. If we take some transition amplitudes (among topological spaces, sets, ...) as specifying a theory, then the choice of a particular differential structure *will* constitute a background since it is also a dynamical entity. We will restrict to manifold category. This also explains why metric by itself is not essential for background independence of gravity, a dynamical tetrad with compatible spin connection would do just as well.

1.3 Towards the construction of a quantum theory

Ultimately constructing a quantum theory of some phenomenon means specifying a state space - (projective) Hilbert space, identifying (self-adjoint) operators on it to correspond to physically observable quantities, a notion of evolution or dynamics such that in a suitable semi-classical approximation, the evolution of expectation values of a class of observables tracks the corresponding classical evolution with the quantum uncertainties less than the observational precision. Here the classical evolution is the one specified by the classical description of the phenomenon. Using such a framework, one can compute matrix elements of suitable observables or transition amplitudes etc. One familiar procedure is that of the *canonical quantization*.

In canonical quantization, typically we have a classical phase space which is cotangent bundle, \mathcal{T}^*Q of some configuration manifold Q and the Hilbert space is the space complex valued functions of Q which are square integrable with respect to some suitable measure, $d\mu$. When $Q \sim \mathbb{R}^N$, we have the familiar $L_2(\mathbb{R}^N, d\mu_{\text{Lebesgue}})$ which is unique thanks to the Stone-von Neumann theorem. This comfortable situation changes once Q becomes topologically non-trivial and/or becomes infinite dimensional. The former can arise due to constraints while the latter arises in a field theory. In relativistic field theory, the *classical configuration space*, Q , is (say) the space of suitably smooth tensor fields which is inadequate to describe the corresponding quantum fields which can be arbitrarily non-smooth. Typically, Q is *extended* to a *quantum configuration space*, \bar{Q} , which should admit a suitable measure.

For a quantum theory of gravity, there are two additional features - (i) we have a theory with first class constraints (i.e. a gauge theory) and (ii) we would like to have background independence.

In presence of constraints, the quantization procedure is a two step process. In the first step one constructs a *kinematical Hilbert space* on which are defined the constraint operators. The second step aims to ‘solve’ the constraints to get a quantum theory corresponding to physical degrees of freedom. Again, *typically*, there are no vectors in the kinematical Hilbert space which are annihilated by the constraint operators and one is forced to consider *distributional solutions*⁵. The space of distributional solution however is *not* a Hilbert space and another inner product needs to be defined on this space to make it into the *physical Hilbert space*. The choice of this inner product is limited by demanding that a suitable class of *Dirac observables* – operators which leave the space of solutions invariant – be self-adjoint.

There are many choices to be made along the way. The requirement of background independence means that no non-dynamical fields should be used in any step. This poses a severe challenge to constructing even the kinematical Hilbert space. The connection formulation of gravity is of great help as the quantum configuration space of a gauge theory, $\overline{\mathcal{A}/\mathcal{G}}$ - space of generalized connections modulo generalized gauge transformations - admits several measures and the demand that the conjugate variables be represented by derivative operators essentially singles out a unique measure - the Ashtekar-Lewandowski measure, essentially constructed from the Haar measure on compact groups. One has a natural choice of Ω and (non-unique) definitions of constraint operators so that the kinematical set-up is well

⁵Let $\Omega \subset H_{\text{kin}}$ be a dense subspace of the kinematical Hilbert space. Let Ω^* denote its algebraic dual (space of linear functions on Ω) so that $\Omega \subset H_{\text{kin}} \subset \Omega^*$. Ω is chosen so that it contains the domains of the constraint operators as well as of other operators of interest. Distributional solutions of constraints are those elements of Ω^* which evaluate to zero on all elements of Ω of the form $\hat{C}|\psi\rangle, \forall \psi \in \Omega$.

founded. We will see the details of these steps.

We will begin with the Hamiltonian formulation of GR in terms of the metric (ADM formulation). Discover the redundant variables and make a canonical transformation to a set of new variables (connection formulation) which are amenable to background independent presentation. These will lead us to the holonomy-flux variables and their Poisson bracket algebra whose representation theory will give us a Hilbert space. This will complete the *first step* in the construction of the quantum theory. Some of its novel features will be revealed through the properties of the geometrical operators. Our study of the basic formalism will conclude with the presentation of the constraint operators on the kinematical Hilbert space. The dynamical aspects will be studied through the simpler cases of homogeneous and isotropic cosmology leading to the Big Bang singularity resolution. The other application of quantum geometry, namely revealing the ‘atoms’ of geometry responsible for the black entropy will be discussed in the second week along with the loop quantum cosmology.

Chapter 2

Classical Hamiltonian Formulation

We are familiar from usual spacial relativistic field theories (say a scalar field) that solutions of the field equations can be viewed as an evolution of fields, their spatial derivatives and their velocities from one spatial slice to another one (“a Cauchy evolution”). In the general relativistic case, one has to deal with space-times other than the Minkowski space-time and eventually make the space-time itself to be ‘dynamical’. However *not all space-times support this notion of evolution*.

To have a well defined, causal (no propagation faster than speed of light in vacuum) and deterministic (given certain data at one instance, the future data is *uniquely* determined), the space-time must be free of *causal pathologies* such as (i) no closed causal (i.e. time-like or null) curves (excludes by *chronology condition*); (ii) no closed causal curves but causal curves which return arbitrarily close to themselves (excluded by *strong causality*); (iii) strong causality holds but when the space-time metric is made slightly ‘wider’, it is violated (excluded by *stable causality*). All such pathologies are absent in space-time which are *stably causal* i.e. admit a differentiable function such that $\partial^\mu f$ is a time-like vector field. This alone is still not sufficient to guarantee the possibility of a *Cauchy Problem*. For this, one needs *Globally Hyperbolic Space-times*. These are space-times which admit a spatial hyper-surface such that events to the future (past) are completely determined by data specified on it. Such space-time admit a globally defined ‘time function’ whose equal time surfaces are Cauchy surfaces. It follows further that such space-times must have the topology: $\mathcal{M} = \mathbb{R} \times \Sigma_3$.

Thus, in order to have a well-posed causal theory of *matter fields*, the space-times must be globally hyperbolic.

It is a non-trivial result of analysis of Einstein equation that Einstein equation can be cast in a Hamiltonian form such that if initial conditions are chosen to satisfy certain *constraints*, then corresponding Hamiltonian evolution generates a solution (space-time) of the Einstein equation¹.

¹This is local existence and uniqueness theorem for the Einstein equation. Since these are short time evolutions, one cannot guarantee that largest possible space-time constructed will be globally hyperbolic. However, if a globally hyperbolic solution is to exist, one can perform a time + space decomposition to put the equations in a Hamiltonian form. That Einstein equation admit a well-posed initial value problem is a necessary condition for globally hyperbolic solutions. That the equations are of Hamiltonian form is an additional, non-trivial property. This follows most directly via the Einstein-Hilbert action formulation.

Although a Hamiltonian formulations can be specified ab initio by giving a *phase space* which is a *symplectic manifold*, a *Hamiltonian* function and specifying evolution by the Hamilton's equations of motion, it is more common that a theory is specified in terms an action which is a functional defined on a set of fields on a space-time manifold. Typically this is expressed as an integral of a Lagrangian density made up of finite order derivatives of a set of tensor (spinor) fields. In such a manifestly space-time covariant presentation, one needs to choose a “time” direction along which to ‘evolve’ data specified on a ‘equal time surface’. These data identify the *configuration space variables and their velocities*. The Hamiltonian formulations is then obtained from this *Lagrangian formulation* by passing through a Legendre transform. This identification of a time direction and a spatial slice on which data are to be specified is referred to as a “3 + 1 decomposition”.

2.1 The 3 + 1 decomposition

Let us assume that our would be space-time manifold is such as to admit a smooth function $T : \mathcal{M} \rightarrow \mathbb{R}$ such that the $T = \text{constant}$ level sets, generate a foliation. Different possible T -functions will generate different foliations. For this to be possible, we must have $\mathcal{M} \sim \mathbb{R} \times \Sigma_3$.

Now choose a vector field $t^\mu \partial_\mu$ which is *transversal* to the foliation i.e. every integral curve of the vector field intersects each of the leaves, transversally. Furthermore, locally in the parameter of the curve, the leaves are intersected once and only once. *Normalize* the vector field so that $t^\mu \partial_\mu T = 1$. This ensures that values of the T -functions can be taken as a “time” parameter which we denote as t .

Fix a leaf Σ_{t_0} and introduce coordinates, $x^a, a = 1, 2, 3$ on it. Carry these along the integral curves of the vector fields, to the other leaves. This sets up a local coordinate system on \mathcal{M} such that the normalized parametrization provides the coordinate t while the integral curves themselves are labelled by the $\{x^a\}$. Note that there is no metric so \mathcal{M} is not yet a space-time. We have only set up a coordinate system.

Choose tensors g_{ab}, N^a, N on each of the leaves in a smooth manner ad *define* a space-time metric via the line element:

$$ds^2 := -N^2 dt^2 + \bar{g}_{ab} (dx^a + N^a dt) (dx^b + N^b dt). \quad (2.1)$$

Choosing \bar{g}_{ab} to be *positive definite* and $N \neq 0$ ensures that the space-time metric $g_{\mu\nu}$ is *invertible*. Its inverse is given by,

$$g^{tt} = -N^{-2}, \quad g^{tb} = N^b N^{-2}, \quad g^{ab} = \bar{g}^{ab} - N^{-2} N^a N^b, \quad \bar{g}^{ac} \bar{g}_{cb} = \delta_b^a. \quad (2.2)$$

We now have a space-time. The space-time metric is defined in terms of 10 independent functions and so there is no loss of generality. It is a convenient parametrization for reasons given below, but alternative parametrization are possible.

It follows that, (i) The induced metric on the leaves is the Riemannian metric \bar{g}_{ab} .

(ii) $n_\mu := \partial_\mu T$ is normal to the leaves, since for any tangent vector $X^\mu \partial_\mu$, to Σ_t , $X^\mu n_\mu = X^\mu \partial_\mu T = 0$. Thanks to the normalization of $t^\mu \partial_\mu$, we have $n_\mu = (1, 0, 0, 0)$.

(iii) $n^\mu := g^{\mu\nu} n_\nu \Rightarrow n^\mu n_\mu = g^{tt} = -N^2 < 0$ and therefore the normal is *time-like* and hence the leaves are *space-like*. The $N n^\mu$ is a unit time-like vector.

(iv) The original transversal vector field can be decomposed as $t^\mu = an^\mu + \tilde{N}^\mu$ where $\tilde{N}^\mu n_\mu = 0$ and hence \tilde{N}^μ is tangential to the leaves and $\tilde{N}^0 = 0$. This decomposition refers to N^2 as the *lapse* function and \tilde{N}^μ as the *shift vector*. Next, $t^\mu n_\mu = 1 \Rightarrow a = -N^2$. The integral curve equation, $d_t x^\mu = -N^2 n^\mu + \tilde{N}^\mu$ implies for $\mu = a$, $\tilde{N}^a = N^2 n^a = N^2 g^{at} = N^2 (N^{-2} N^a) = N^a$. This identifies the N^a with the shift vector (which is spatial).

The particular parametrization of the space-time metric can be said to be *adapted* to the pre-selected coordinate system. Since the coordinate system is defined *without* any reference to any metric, we can similarly parametrize other tensor fields, notably the *co-tetrad*, e_μ^I .

Note: We chose an arbitrary foliation (through an arbitrary choice of a “Time” function and then a transversal vector field to enable us to choose coordinate on the manifold. The foliation provides us with a normal n_μ and the transversal vector field can be parametrized in terms of this normal, a lapse function and a shift vector. Varying the lapse and shift varies the transversal vector field *relative to the foliation*. If we also change the foliation, then the normal changes and so must the shift vector. The changes induced by lapse and shift correspond to making a space-time diffeomorphism and *every infinitesimal space-time diffeomorphism can be generated by infinitesimal changes in the lapse and shift*.

2.2 Digression on tetrad formulation

General relativity is formulated as theory consisting of tensorial fields on a manifold and a second rank, symmetric, non-degenerate (invertible) tensor field, $g_{\mu\nu}$ encoding gravitational phenomena. To do differential calculus on general tensor fields one also needs to define a covariant derivative, ∇_μ which involves the introduction of an affine connection, $\Gamma^\lambda_{\mu\nu}$, which is usually taken to symmetric and *metric compatible* i.e. $\nabla_\lambda g_{\mu\nu} = 0$. The non-abelian gauge theories already introduce quantities which are not just tensors with respect to general coordinate transformations but also transform under the action of “an internal” group, eg a Higgs field Φ^a , a YM potential A_μ^a , its corresponding field strength, $F_{\mu\nu}^a$ etc. The index a indicates a response to the (adjoint) action of a group such as $SU(N)$. Developing calculus for such quantities, also needs a *gauge* covariant derivative and a corresponding *gauge* connection eg A_μ^a .

Consider now a quantity, $e_\mu^I(x)$ where μ responds to a general coordinate transformation (e_μ^I transform as a covariant rank 1 tensor) and the index I responds to the *local* action of the pseudo-orthogonal group, $SO(1,3)$ under the defining representation. This quantity can also be thought of as a 4×4 matrix and we will take it to be an invertible matrix. This is referred to as a *co-tetrad* while its inverse quantity, e_I^μ is referred to as a *tetrad*: $e_\mu^I e_J^\mu = \delta_J^I$, $e_\mu^I e_I^\nu = \delta_\mu^\nu$. It is possible to formulate the theory of gravity in terms of a (co-)tetrad as follows.

(1) Let $\Lambda_J^I \in SO(1,3)$ i.e. $\Lambda_K^I \Lambda_L^J \eta^{KL} = \eta^{IJ}$ holds where $\eta^{IJ} = \text{diag}(-1, 1, 1, 1)$. Then the co-tetrad transforms as:

$$(e')_\mu^I(x'(x)) := \Lambda_J^I(x) \frac{\partial x'^\nu}{\partial x^\mu} e_\nu^J(x). \quad (2.3)$$

The Λ - transformation is referred to as a *Local Lorentz Transformation* (LLT) while $x \rightarrow x'(x)$ is the *General Coordinate Transformation* (GCT). Clearly to have the derivatives of the co-tetrad to transform covariantly under both sets of transformations, we need two connections: an *affine connection* (not necessarily symmetric in the lower indices) and a *Spin connection*, ω_μ^{IJ} . The spin connection is anti-symmetric in the IJ indices and thus

transforms as the *adjoint representation* of the pseudo-orthogonal group. The derivative covariant with respect to the LLT is denoted by D_μ , that with respect to GCT is denoted by the usual ∇_μ while the one with respect to both will be denoted by \mathcal{D}_μ . The Lorentz indices will be raised/lowered using the *Lorentz metric* η^{IJ}, η_{IJ} , where $\eta^{IK}\eta_{KJ} = \delta^I_J$.

Armed with the tetrad, the spin connection and the Lorentz metric, *define* the following quantities:

Torsion :	$T^I(e, \omega) := de^I + \omega^I{}_J \wedge e^J$ $T^I{}_{\mu\nu} = \partial_\mu e^I_\nu + \omega_\mu{}^I{}_J e^J_\nu - (\mu \leftrightarrow \nu)$
Curvature :	$R^{IJ}(\omega) := d\omega^{IJ} + \omega^I{}_K \wedge \omega^{KJ}$ $R^{IJ}{}_{\mu\nu} = \partial_\mu \omega_\nu{}^{IJ} + \omega_\mu{}^I{}_K \omega_\nu{}^{KJ} - (\mu \leftrightarrow \nu)$
Bianchi Identity :	$(DR)^I{}_J = 0 := dR^I{}_J + \omega^I{}_K \wedge R^K{}_J + \omega_J{}^K \wedge R^I{}_K$
Cyclic Identity :	$(DT)^I = R^I{}_J \wedge e^J := dT^I + \omega^I{}_J \wedge T^J$
Metric :	$g_{\mu\nu}(e, \eta) := e^I_\mu e^J_\nu \eta_{IJ}$
Christoffel Connection :	$\left\{ \begin{array}{c} \lambda \\ \mu\nu \end{array} \right\} (g(e)) := \frac{1}{2} g^{\lambda\alpha} (g_{\alpha\mu, \nu} + g_{\alpha\nu, \mu} - g_{\mu\nu, \alpha})$
Affine connection : where,	$\Gamma^\lambda{}_{\mu\nu}(e, \omega) := \left\{ \begin{array}{c} \lambda \\ \mu\nu \end{array} \right\} (g(e)) + \frac{1}{2} g^{\lambda\alpha} (T_{\alpha\mu\nu} - T_{\mu\nu\alpha} - T_{\nu\mu\alpha})$ $\mathbf{T}_{\alpha\mu\nu}(\mathbf{e}, \omega) := \mathbf{e}_{I\alpha} \mathbf{T}^I{}_{\mu\nu}(\mathbf{e}, \omega)$
These imply	
Matric compatibility : tetrad compatibility :	$\nabla_\lambda g_{\mu\nu} = 0$ $\mathcal{D}_\mu e^I_\nu = 0 := \nabla_\mu e^I_\nu + \omega_\mu{}^I{}_J e^J_\nu - \Gamma^\lambda{}_{\mu\nu} e^I_\lambda$
Compatibility \Rightarrow	$R^\alpha{}_{\lambda\mu\nu}(\Gamma) = e_I^\alpha e_{\lambda J} R^{IJ}{}_{\mu\nu}(\omega)$

No assumption about the torsion tensor is made.

(2) It is possible to invert the torsion equation to ‘solve for’ the spin connection in terms of the tetrad, its derivatives and the torsion tensor. All one needs to do is manipulate the combination $T_{\lambda\mu\nu} + T_{\mu\nu\lambda} - T_{\nu\lambda\mu}$ and use the invertibility of the (co-)tetrad. The result is:

$$\omega_\mu{}^{IJ} := \hat{\omega}_\mu{}^{IJ}(e) + K_\mu{}^{IJ}(e, T) \quad (2.4)$$

$$\hat{\omega}_\mu{}^{IJ} := \frac{1}{2} [e^{\nu I} (\partial_\mu e_\nu^J - \partial_\nu e_\mu^J) - e^{\nu J} (\partial_\mu e_\nu^I - \partial_\nu e_\mu^I) - e^{\nu I} e^{\lambda J} (\partial_\nu e_\lambda^K - \partial_\lambda e_\nu^K) e_{\mu K}] \quad (2.5)$$

$$K_\mu{}^{IJ} := -\frac{1}{2} e^{\nu I} e^{\lambda J} (T_{\nu\lambda\mu} + T_{\lambda\mu\nu} - T_{\mu\nu\lambda}) \quad (2.6)$$

The K is called the *con-torsion tensor* and $\hat{\omega}$ is the *torsion-free spin connection* which is explicitly determined by the tetrad. The Affine connection equation is the corresponding inversion of the metric compatibility condition (covariant constancy of the metric) to express the general affine connection in terms of the torsion free Christoffel connection plus the torsion combinations.

Notice that a priori, we have two connections: the affine and the spin. Both define corresponding and independent torsions ($T^I{}_{\mu\nu}$ and the antisymmetric part of $\Gamma^\lambda{}_{\mu\nu}$). The introduction of the metric as the ‘square’ of the co-tetrad and the two compatibility conditions together identify the two torsions.

The last equation demonstrates that we can use the tetrad and the co-tetrad to convert the Lorentz indices and the general tensor indices into each other with the compatibility conditions ensuring the two distinct curvatures also going into each other.

Although we have referred to only 4 dimensions and Lorentz signature metric, the definitions generalise to any dimensions and any signature.

(3) Four dimensions have additional features available. One can define *internal dual* (Lorentz dual) for anti-symmetric rank-2 Lorentz tensors apart from the usual *Hodge dual* (space-time dual) for 2-forms.

Let, \mathcal{E}^{IJKL} and $\mathcal{E}_{\mu\nu\alpha\beta}$ denote the Levi-Civita symbols; These are completely antisymmetric in their indices and we choose the conventions: $\mathcal{E}^{0123} = 1 = \mathcal{E}_{txyz}$. The indices on these are raised and lowered by the Lorentz and the space-time metric respectively. Using these we define:

$$\tilde{X}^{IJ} := \frac{1}{2} \mathcal{E}^{IJ}{}_{KL} X^{KL} \quad (\text{Internal Dual}) \quad (2.7)$$

$$(*X)_{\mu\nu} := \frac{1}{2} \mathcal{E}_{\mu\nu}{}^{\alpha\beta} X_{\alpha\beta} \quad (\text{Hodge Dual}) \quad (2.8)$$

(4) From the tetrad and the spin connection, the following Local Lorentz invariant four forms can be constructed whose integrals are candidate terms for an action.

1. *Hilbert-Palatini*: $\mathcal{L}_{HP}(e, \omega) := \frac{1}{2} \mathcal{E}_{IJKL} R^{IJ}(\omega) \wedge e^K \wedge e^L$.

The variational equations following from this are equivalent to the Einstein equations. The spin-connection equation implies that the torsion vanishes and the tetrad equation implies the vanishing of the Ricci tensor. The Hilbert-Palatini action is thus classically equivalent to the Einstein-Hilbert action of the metric formulation.

This term taken as an action with the tetrad and spin connection treated as independent variables is sometimes referred to as the tetrad formulation of gravity.

2. *Cosmological Constant*: $\mathcal{L}_\Lambda(e) := \frac{\Lambda}{4!} \mathcal{E}_{IJKL} e^I \wedge e^J \wedge e^K \wedge e^L$

This is the usual cosmological constant term, proportional to the volume form.

3. *Euler Invariant*: $\mathcal{L}_E(\omega) := \frac{1}{2} \mathcal{E}_{IJKL} R^{IJ} \wedge R^{KL}$.

This 4-form is a *topological term* i.e. its variation under arbitrary infinitesimal changes in the spin connection, is an exact form and therefore the variation of its integral receives contributions only from the *boundary values*. Furthermore, explicitly,

$$\mathcal{L}_E(\omega) = -d \left\{ \frac{1}{2} \mathcal{E}^I{}_{JMN} \omega^{MN} \wedge \left(d\omega^J{}_I + \frac{2}{3} \omega^J{}_K \wedge \omega^K{}_I \right) \right\} \quad (2.9)$$

4. *Pontryagin Invariant*: $\mathcal{L}_P(\omega) := R^{IJ} \wedge R^{IJ}$.

This 4-form is also a *topological term*. Furthermore, explicitly,

$$\mathcal{L}_P(\omega) = -d \left\{ \omega^I{}_J \wedge \left(d\omega^J{}_I + \frac{2}{3} \omega^J{}_K \wedge \omega^K{}_I \right) \right\} \quad (2.10)$$

The terms enclosed within the braces is the *Chern-Simmons* 3-form.

5. *Nieh-Yan Invariant*: $\mathcal{L}_{NY}(e, \omega) := T^I \wedge T_I - R^{IJ} \wedge e^I \wedge e^J$.

This 4-form is also a *topological term* which depends on both the tetrad and the spin connection. It vanishes if torsion is zero (for zero torsion, the second term vanishes by the cyclic identity.) Explicitly,

$$\mathcal{L}_{NY} = d \{ e_I \wedge T^I \}. \quad (2.11)$$

Note that we have 5 different, Lorentz covariant 2-forms: $T^I, \Sigma^{IJ} := e^I \wedge e^J, \tilde{\Sigma}^{IJ}, R^{IJ}, \tilde{R}^{IJ}$. From these, we can form the six Lorentz invariants: $T^2, \Sigma^2 (= 0 = -\tilde{\Sigma}^2), \Sigma \wedge \tilde{\Sigma}, R^2 (= -\tilde{R}^2), R \wedge \tilde{R}, R \wedge \Sigma, R \wedge \tilde{\Sigma}$. If we are to get the Einstein equation (with a cosmological constant), then the T^2 and $R \wedge \Sigma$ must be combined into the Nieh-Yan combination,

(5) We will note a parametrization of the tetrad, adapted to the 3+1 decomposition, which leads to the corresponding metric decomposition. This can be derived from the identifications:

$$\begin{aligned} e_t^I e_t^J \eta_{IJ} &:= -N^2 + \bar{g}_{ab} N^a N^b \\ e_t^I e_a^J \eta_{IJ} &:= \bar{g}_{ab} N^b \\ e_a^I e_b^J \eta_{IJ} &:= \bar{g}_{ab} \end{aligned} \quad (2.12)$$

It follows,

<p>Co – tetrad :</p> $e_t^I := N n^I + N^a V_a^I$ $e_a^I := V_a^I \quad (\text{free})$ $\bar{g}_{ab} := V_a^I V_b^J \eta_{IJ}$	<p>Introduces n_I</p> $n^I n^J \eta_{IJ} := -1 \quad , \quad n^I V_a^J \eta_{IJ} = 0$ <p>is invertible;</p>
<p>Tetrad :</p> $e_t^t := -N^{-1} n_I$ $e_I^a := N^{-1} n_I N^a + V_I^a$	<p>Defines V_I^a</p> $n^I V_I^a := 0$ $V_I^a V_b^I = \delta_b^a \quad , \quad V_I^a V_a^J = \delta_I^J + n_I n^J$

In this parametrization, the 16 variables in the tetrad have been traded with $V_a^I(12)$, N , $N^a(4)$ and $n^I(4)$ variables with 4 conditions: $n^2 = -1$, $n \cdot V_a = 0$. The conditions can be viewed as 4 conditions on n^I given freely chosen V_a^I or one condition on n^I and 3 conditions on V_a^I given freely chosen spatial vector n^i .

Notice that we have the *normalized normal*, Nn_μ defined by the foliation. From this we can construct an internal vector $\tilde{n}^I := e_I^\mu(Nn_\mu)$. In the parametrization, we have also introduced an internal normalized time-like vector n^I , determined by the freely chosen V_a^I . These two are related by the parametrization of the tetrad as, $\tilde{n}^I = -n^I$.

We can view n_μ defined by the foliation and n_I defined by a choice of V_a^I as two time-like normalized vectors in the $T^*(\mathcal{M})$. These are not identical in general and in particular n_I is not normal to the foliation. Demanding it to be so, puts a restriction on the V_a^I : $n_I \propto n_\mu \Rightarrow n_i = 0$, $n_0 n^0 = -1$ and $n \cdot V_a = 0 \Rightarrow V_a^0 = 0$. This implies that V_a^I are confined to $T^*(\Sigma)$. This choice is the so-called *time gauge*.

Finally, we reiterate that using the tetrad and co-tetrad we can freely convert the Lorentz and the general coordinate indices into each other. The normalized normal (Nn_μ) can be used to define a *projector*, $P_\nu^\mu := \delta_\nu^\mu + N^2 n^\mu n_\nu$ which projects space-time tensors onto *spatial tensors*. This would lead to 3+1 decomposition (or parametrization) of all other tensorial quantities.

Chapter 3

Symmetry Reduction

There are different uses of the term ‘symmetry reduction’. Heuristically, if S is a state space of a system, on which is specified an action of a group, G , which preserves the defining specification of the system (so that G is its *symmetry group*), then the space S gets “decomposed” into orbits of G . The space of orbits, S/G , is ‘smaller’ than S and could constitute a simplification. S/G , is thought of as a *symmetry reduction of S by G* . Alternatively, one could restrict to the subset of the so called *invariant* states which may be thought of as a collection of trivial orbits. In our context, we will be using the term in the latter sense. The system could be classical or quantum mechanical.

For example, if S is the quantum mechanical state space of a particle with a rotationally invariant Hamiltonian, then the subspace of the invariant states would be all the states with zero angular momentum. If it is the phase space of a particle with a rotationally invariant dynamics, then the only invariant ‘state’ is the origin of the configuration space with zero momentum. If however, S denotes the space of field configurations on a manifold, then the subset of invariant configurations is non-trivial. If the quantum mechanical state space of a system consists of *distributions* on a space of ‘test functions’, then invariant states could be defined as those distributions whose support consists of invariant test functions.

If one obtains a reduction by restricting to invariant states (and invariant observables) of a quantum system, one has followed the *first quantize, then reduce* route and the reduced system can be thought of as a *symmetric sector*. This is not always possible, since one does not have adequate explicit control over the quantum system. Alternatively, one can consider invariant subspace of a classical phase space and construct a corresponding quantum theory. This is the *first reduce, then quantize* route. In general, the relation between these two approaches is unclear.

While the former approach is more desirable, in practice, it is the latter approach which is followed commonly. We will also follow this approach. However, we will follow the methods – basic variables, construction of quantum Hilbert space etc – used in the full theory. The viability of these simplified models are then thought to constitute a test of the methods and premises of the full theory. The reduction of the classical theory is carried out by requiring certain *symmetries* to be exactly realized.

3.1 Symmetry Reduced Models

We are already familiar with use of symmetries to simplify a problem. For example, assuming spherical symmetry we choose coordinates and metric components to simplify the Einstein equation and obtain the Schwarzschild solution or using homogeneity and isotropy one obtains the FRW solutions. Thus symmetry groups (isometries) allow us to classify suitable ansatz for the basic variables of the theory. Note however that we are not interested in solving Einstein equations, but rather in obtaining a classical action with fewer degrees of freedom and constructing a corresponding quantum theory. In the context of spherical symmetry for example, this corresponds to restricting to only spherically symmetric form of 3-metrics: $ds^2 = \Lambda^2(t, r)dr^2 + R^2(t, r)(d\theta^2 + \sin^2\theta d\phi^2)$ and reducing the Einstein-Hilbert action to get an action in terms of the two field degrees of freedoms – $\Lambda(r), R(r)$. Such reductions of degrees of freedom is termed *mini-superspace* model if the degrees of freedom is *finite* and a *midi-superspace* model, if the degrees of freedom is still infinite i.e. a lower dimensional field theory. The former occur in *homogeneous cosmologies* while examples of the latter include spherical symmetry, certain inhomogeneous cosmological models such as the Gowdy models, Einstein-Rosen waves etc. Needless to say that the midi-superspace models are still very complicated. We will concentrate on the mini-superspace models and specifically on (spatially) homogeneous cosmologies. We begin by defining spatially homogeneous space-times which are not necessarily solutions of Einstein equation.

3.1.1 Spatially homogeneous models

A four dimensional space-time is said to be spatially homogeneous if (a) it can be foliated by a 1-parameter family of space-like hypersurfaces, Σ_t and (b) possessing a (Lie) group of isometries such that for each t and any two points $p, q \in \Sigma_t$ there exist an isometry of the space-time metric which maps p to q . The isometry group G is then said to act *transitively* on each of the Σ_t . If the group element connecting p, q is unique, the group action is said to be *simply transitive* (otherwise multiply transitive). Spatially homogeneous space-times are further divided into two types.

A spatially homogeneous space-time is said to be of a **Bianchi type** if the group of isometries contains a subgroup (possibly itself), G^* , which acts simply transitively on Σ_t otherwise it is said to be of the **Kantowski-Sachs type** (interior of Schwarzschild solution). It turns out that except for the special case of $\Sigma \sim S^2 \times \mathbb{R}$ and $G = SO(3) \times \mathbb{R}$, in all other cases one has a Bianchi type space-time.

Transitive action implies that there must be at least three independent Killing vectors at each point of Σ_t since Σ_t is three dimensional. But there could be additional Killing vectors which vanish at a point. These Killing vectors generate the *isotropy* (or stability) subgroup, H of G . Since H will induce a transformation on the tangent spaces to the spatial slices, it must be a subgroup of $SO(3)$ and thus dimension of G can be at most 6 and at least 3 since the dimension of G^* is always 3. All 3 dimensional Lie groups have been classified by Bianchi into 9 types. The classification goes along the following lines[3].

A Lie algebra (or connected component of a Lie group) is characterised by structure constants

C^I_{JK} with respect to a basis X_I , satisfying the antisymmetry and Jacobi identity namely,

$$[X_J, X_K] = C^I_{JK} X_I ; C^I_{JK} = C^I_{KJ} ; \sum_{(IJK)} C^N_{IL} C^L_{JK} = 0 , I, J, K = 1, 2, 3 .$$

Using the availability of the Levi-Civita symbols, \mathcal{E}_{IJK} , \mathcal{E}^{IJK} , $\mathcal{E}_{123} = 1 = \mathcal{E}^{123}$, we can write the structure constants as,

$$C^I_{JK} = \mathcal{E}_{JKL} C^{LI} , C^{IJ} := M^{IJ} + \mathcal{E}^{IJK} A_K \quad (3.1)$$

Thus, the 9 structure constants are traded for 6 M^{IJ} (symmetric in IJ) and the 3 A_K . This has used only antisymmetry. The Jacobi identity implies, $M^{IJ} A_J = 0$.

Noting that the structure constants are subject to linear transformations induced by linear transformations, $X_I \rightarrow S_I^J X_J$, on the basis of the Lie algebra, the symmetric M^{IJ} can be diagonalized by orthogonal transformations and the non-zero eigenvalues can be further scaled to ± 1 : $M^{IJ} = n^I \delta^{IJ}$. The condition $M^{IJ} A_J = 0$ implies that *either* $A_I = 0$ (**Class A**) *or* $A_I \neq 0$ (**class B**) in which case M^{IJ} has a zero eigenvalue and we may take the non-zero eigenvector A_I to be along the ‘‘1st’’ axis, i.e. $A_I = a \delta_{I,1}$ and $n^1 = 0$. This leads to,

$$[X_J, X_K] = n^I \mathcal{E}_{IJK} X_I + X_J A_K - X_K A_J .$$

In the class A, there are precisely 6 possibilities organized by the *rank of the matrix* – 0, 1, 2, 3 and *signature* for ranks 2, 3 viz $(+, +, +)$ and $(+, +, -)$. The eigenvalues of M^{IJ} can be taken to be $n^I = \pm 1, 0$.

In the class B, the rank of M^{IJ} cannot be 3 and the possibilities are restricted to the ranks 0, 1, 2 and signatures $(+, +, +)$ for rank 2. If the rank of M is 0, all three eigenvalues are zero and scaling X_1 , we can arrange $a = 1$. For rank 1, taking n_3 to be the non-zero eigenvalue, scaling X_1, X_3 ensures $a = 1$. For rank 2 however, $(n_2 = \pm 1, n_3 = \pm 1)$, no scaling can preserve n_2, n_3 and set $a = 1$ (of course $a = 1$ is possible).

Here is a table of the classification of Riemannian, homogeneous 3-geometries[3]:

Type	a	n_1	n_2	n_3	Remarks
Class A					
I	0	0	0	0	Euclidean space
					(Leads to the Kasner space-time)
II	0	1	0	0	
VII ₀	0	1	1	0	
VI ₀	0	1	-1	0	
IX	0	1	1	1	S^3 is a special case (with isotropy)
					(Central to BKL Scenario)
VIII	0	1	1	-1	
Class B					
V	1	0	0	0	H^3 a special case (with isotropy)
IV	1	0	0	1	
VII _a	a	0	1	1	
III	1	0	1	-1	sub-case of type VI _a
VI _a	a	0	1	-1	

Of interests to us are the so called *class A* models which are characterised by the structure constants satisfying $C^I{}_{IJ} = 2A_J = 0$ ¹.

When $H = SO(3)$, one has homogeneity *and* isotropy i.e. FRW space-times. We know that these come in three varieties depending on the constant spatial curvature. The spatially flat case is of type Bianchi I while positively curved case is of type Bianchi IX. (The negatively curved case is in class B, type V).

The metrics of the general Bianchi type space-times have at the most 6 degrees of freedom thus constituting mini-superspaces. The spatial metrics *can be put* in the form: $ds^2 = g_{IJ}(t)e_i^I e_j^J dx^i dx^j$, where $e_i^I dx^i$ are the so called Maurer-Cartan forms on the group manifold G^* , satisfying $de^I = -\frac{1}{2}C_{JK}^I e^J \wedge e^K$. When one further restricts to *diagonal* g_{IJ} one gets the so-called *diagonal Bianchi models*.

Remark: One should notice that restricting to a subclass of metrics amounts to introducing *background structures* from the perspective of the full theory. In the present case, these structures are the symmetry group and the coordinates adapted to the group action (which allowed the metric to be put in the specific form). This is unavoidable and constitutes a specification of the reduced model. From the perspective of a reduced model, these structures are *non-dynamical, analogous to the manifold structure for the full theory* and therefore do not automatically violate background independence. Instead, the background independence now means that quantization procedure should not depend the metric g_{IJ} which is a dynamical variable.

Our basic variables however are not the 3-metric and the extrinsic curvatures. They are the $SU(2)$ connection and the densitized triad. In the metric variables, the natural notion of symmetry is isometry while in the connection formulation it is the *group of automorphisms* of the $SU(2)$ bundle. Thus, the cosmological models will now be understood to be characterised by groups of automorphisms of the $SU(2)$ bundle which acts on the base manifold Σ transitively. The task is to characterise the connection and triad variables which are *invariant* under the group action (just as isometries mean invariant metrics). This requires more mathematical machinery and we will only state the conclusions².

For the Bianchi models, the invariant connections and densitized triad are of the form:

$$A_a^i(t, x) := \Phi_I^i(t)\omega_a^I(x) \quad , \quad E_i^a(t, x) := \sqrt{g_0}(x)p_i^I(t)X_I^a(x). \quad (3.2)$$

In the above equation, a refers to spatial coordinate index, i refers to the adjoint representation of $SU(2)$ and I refers to the adjoint index of the Lie algebra of the symmetry (sub) group G^* (and hence takes 3 values). The $\omega_a^I dx^a$ are the Maurer-Cartan 1-forms (left-invariant 1-forms) on Σ_t identified with the group manifold while $X_I^a \frac{\partial}{\partial x^a}$ are the corresponding invariant vector fields dual to the 1-forms, i.e. $\omega^I(X_J) = \omega_a^I X_J^a = \delta_J^I$. The $g_0(x)$ is the determinant of the invariant metric on the symmetry group and provides the necessary density weight. It is regarded as a fiducial quantity and will drop out later. All the coordinate dependence resides in these forms, vector fields and the fiducial metric while the coefficients containing the t dependence are the basic dynamical variables³.

¹The remaining, Class B models are thought not have a Hamiltonian formulation and hence are not amenable to analysis by canonical methods [4].

²A few essential details from Forgacs and Manton are summarised in the appendix.

³Similar decomposition is made for all quantities with spatial and the Lorentz indices. The *contravariant* spatial index is expressed using the invariant vector fields and the covariant one using the invariant 1-forms. In particular, $K_a^i := K_I^i \omega_a^I$, $\Gamma_a^i := \gamma_I^i \omega_a^I$.

If we have isotropy in addition, then the degrees of freedom are further reduced: $\Phi_I^i := c\Lambda_I^i$, $p_i^I := p\Lambda_i^I$ and there is only one degree of freedom left. Here the Λ 's are a set of orthonormal vectors satisfying, $\Lambda_I^i\Lambda_J^i = \delta_{IJ}$, $\Lambda_I^i\Lambda_J^j\Lambda_K^k\epsilon_{ijk} = \epsilon_{IJK}$. The phase space variables c, p are gauge invariant.

The intermediate case of *diagonal models* arises from a choice $\Phi_I^i := c_I\Lambda_I^i$, $p_i^I := p^I\Lambda_i^I$ (no sum over I). The residual (SU(2)) gauge transformations act on the Λ 's and leaving the c_I, p^I as the *gauge invariant* phase space variables thereby solving the Gauss constraint at the outset⁴. Thus there are only 3 degrees of freedom [5].

Having identified relevant degrees of freedom parameterising quantities invariant under symmetry transformation, the next task is to obtain the symplectic structure (basic Poisson brackets) and simplify the expressions for the constraints.

Symplectic form: In the full theory, this is given by $(8\pi G\gamma)^{-1} \int_{\Sigma} d^3x \dot{A}_a^i(t, x) E_i^a(t, x)$. Direct substitution gives,

$$\frac{1}{\kappa\gamma} \int_{\Sigma} d^3x \dot{A}_a^i(t, x) E_i^a(t, x) = \frac{1}{\kappa\gamma} \dot{\Phi}_I^i p_i^I \left\{ \int_{\Sigma} d^3x \sqrt{g_0} \right\}, \Rightarrow \{\Phi_I^i, p_j^J\} = \frac{\kappa\gamma}{V_0} \delta_j^i \delta_I^J. \quad (3.3)$$

The quantity in the braces is the *fiducial* volume, V_0 , of Σ_t . For spatially flat, isotropic case, the slice is non-compact and the fiducial volume is infinite. This problem is addressed by restricting to a finite cell whose fiducial volume is finite. One has to ensure that the final results do *not* depend on the fiducial cell⁵. The dependence on the fiducial volume is gotten rid off by redefining the basic variables as $\Phi \rightarrow \Phi V_0^{-1/3}$, $p \rightarrow p V_0^{-2/3}$. If we have isotropy, the symplectic form would become $\frac{3}{\kappa\gamma} V_0 \dot{c} p$ which leads to (after rescaling) to the Poisson bracket, $\{c, p\} = \frac{\kappa\gamma}{3}$. With this rescaling understood, we will now effectively put $V_0 = 1$.

Curvature: The curvature corresponding to the invariant connection above, is obtained as:

$$F^i := dA^i + \frac{1}{2} \epsilon^i{}_{jk} A^j \wedge A^k := \frac{1}{2} F_{JK}^i \omega^J \wedge \omega^K \quad (3.4)$$

$$\therefore F_{JK}^i = -\Phi_I^i C^I{}_{JK} + \epsilon^i{}_{jk} \Phi_J^j \Phi_K^k \quad (3.5)$$

Gauss Constraint: The full theory expression is:

$$\begin{aligned} G(\Lambda) &:= \int_{\Sigma} \Lambda^i \left\{ \frac{1}{\kappa\gamma} (\partial_a E_i^a + \epsilon_{ij}{}^k A_a^j E_k^a) \right\} \\ &= \frac{\Lambda^i}{\kappa\gamma} \left[\underbrace{p_i^I \int_{\Sigma} \partial_a (\sqrt{g_0} X_I^a)}_{-V_0 C^J{}_{IJ}} + \epsilon_{ij}{}^k p_k^I \Phi_J^j \underbrace{\int_{\Sigma} \sqrt{g_0} X_I^a \omega_a^J}_{V_0} \right] \end{aligned} \quad (3.6)$$

$$\therefore G_i = (\kappa\gamma)^{-1} \{-p_i^I C^I{}_{IJ} + \epsilon_{ij}{}^k \Phi_I^j p_k^I\}. \quad (3.7)$$

Notice that for the class A models, the first term is zero and for the *diagonal* models the second term vanishes as well (since ϵ is antisymmetric in j, k while the Λ factors are symmetric in j, k). There are no continuous gauge invariances left. Note that the first term in eqn (3.7),

⁴There is still a discrete invariance remaining and involves changing the sign of two of the triad and connection components.

⁵This is discussed in more details in section 4.2.2

is a surface term which *could* vanish if Σ has no boundaries. But this would not be true for say spatially flat models which will have the Σ as a cell on which the invariant vector fields need not vanish. The integrand however is proportional to C^J_{IJ} and these vanish for the class A models.

Diffeo Constraint:

$$C_{\text{diff}}(\vec{N}) := \frac{1}{\kappa\gamma} \int_{\Sigma} N^a(x) E_i^b(x) F_{ab}^i(x) - \int_{\Sigma} N^a(x) A_a^i(x) G_i(x)$$

$$N^a(t, x) := N^I(t) X_I^a(x) \quad (3.8)$$

$$\therefore N^I C_I = \frac{N^I}{\kappa\gamma} [(C^K_{JK} \Phi_I^i + C^K_{IJ} \Phi_K^i) p_i^J] \quad (3.9)$$

This constraint again vanishes for *diagonal*, class A models.

Hamiltonian Constraint: The full theory Hamiltonian constraint is given by,

$$C_{\text{Ham}}(N) := \frac{1}{2\kappa} \int_{\Sigma} N \frac{E_i^a E_j^b}{\sqrt{|\det q|}} [\epsilon^{ij} F_{ab}^k - 2(1 + \gamma^2) K_{[a}^i K_{b]}^j] \quad (3.10)$$

To carry out the integration, we need to note the expressions:

$$\sqrt{g_0} = \frac{1}{3!} \epsilon_{IJK} \epsilon^{abc} \omega_a^I \omega_b^J \omega_c^K, \quad \frac{1}{\sqrt{g_0}} = \epsilon_{abc} \epsilon^{IJK} X_I^a X_J^b X_K^c. \quad (3.11)$$

This leads to,

$$\det q = \det(E_i^a) := \frac{1}{3!} \epsilon_{abc} \epsilon^{ijk} (g_0)^{3/2} X_I^a X_J^b X_K^c p_i^I p_j^J p_k^K = \frac{1}{3!} g_0 \epsilon^{ijk} \epsilon_{IJK} p_i^I p_j^J p_k^K \quad (3.12)$$

Now the integration can be carried out immediately to give,

$$H_{\text{grav}} = \frac{N}{2\kappa} \left[\frac{p_i^I p_j^J}{\sqrt{\frac{1}{6} |\epsilon^{ijk} \epsilon_{IJK} p_i^I p_j^J p_k^K|}} \left\{ \epsilon^{ij} k F^k_{IJ} - 2(1 + \gamma^2) K_I^{[i} K_J^{j]} \right\} \right] \quad (3.13)$$

In the above, $K_I^i = \gamma^{-1}(\Phi_I^i - \Gamma_I^i)$. These expressions are valid for general Bianchi models.

At this stage, we could in principle attempt to carry out the usual Schrodinger quantization with Φ_I^i being multiplicative operators and P_i^I being the derivative operators. Both transform covariantly under the action of SU(2).

However, we can also imagine ‘specializing the holonomy-flux variables’ of the full theory, for these symmetric fields. It is natural to choose edges along the symmetry directions i.e. along integral curves of the X_I^a vector fields. It follows that due to homogeneity, the path ordered exponentials, holonomies, become just the *ordinary exponentials*, $h_I(\Phi) := h_{e_I}(\Phi) := \mathcal{P} \exp\{\int_{e_I} \Phi_I^i \tau_i \omega_a^I dx^a\} = \exp\{\Phi_I^i(t) \tau_i \int_{e_I} \omega_a^I dx^a\}$. There is no sum over I in these expressions. These can be further expressed using the identity $e^{i\theta \hat{n} \cdot \vec{\sigma}} = \cos(\theta) + i \hat{n} \cdot \vec{\sigma} \sin\theta$. The holonomy is then given in terms of $\theta \sim \sqrt{\Phi_I^i \Phi_I^i}$ which is gauge invariant and two angular, gauge variant components corresponding to the direction $\hat{n} \sim$ unit vector in the direction of Φ_I^i . A simplification occurs if we further restrict to the diagonal models: $\Phi_I^i := c_I \Lambda_I^i$ which makes the $\hat{n} = \vec{\Lambda}_I$ and now the matrix elements of these holonomies can be obtained from the elementary functions, $e^{\mu^{(I)} c_I/2}$. These have been termed as the *point holonomies*.

The fluxes through surfaces perpendicular to the symmetry directions, likewise simplify to $E_{S_{JK}}(f) = p^I \Lambda_i^I f^i \int_{S_{JK}} \sqrt{g_0(x)} \epsilon_{abc} X_I^a dS^{bc} \propto p^I$. Unlike the flux operators in the full theory, these fluxes Poisson commute among themselves. Thus, in the diagonal models, we can extract gauge invariant phase space coordinates, with the holonomies and fluxes having the usual Poisson algebra. In quantum theory, a useful triad representation can then be set-up.

Point holonomies and commuting flux variables are new features which arise in the (diagonal) mini-superspace reduction. These are also responsible for the relative ease of analysis possible for these models. This will be discussed more below.

What about inhomogeneous models? There have fewer efforts regarding these. Among the inhomogeneous models, the reduction for the Gowdy model on 3-torus can be seen in [6], while spherical symmetric model can be seen in [7]. Martin's lattice model is briefly discussed in the appendix.

Chapter 4

Singularity Resolution in Quantum Theory

The most detailed analysis of the singularity resolution is available for the homogeneous and isotropic geometry coupled to a massless scalar and this is the case that we discuss below. Prior to 2005, the singularity resolution was understood as the deterministic nature of fundamental equation (the Hamiltonian constraint) and in terms of an effective picture deduced either from the WKB approximation or by taking expectation values of the Hamiltonian. In this sense, resolution of singularities was seen for (i) FRW coupled to a scalar field with arbitrary positive semidefinite potential and (ii) diagonalised Bianchi class A (anisotropic) models. These resolutions were seen as an implication of the *inverse triad quantum corrections* which were present in the matter sector (and in the curvature for non-flat models). Post 2005, it was realized, at least for the FRW case, that *the holonomy corrections by themselves could also resolve singularities*. This required restriction to massless scalar and treating it as a clock variable, thereby paving the way for construction of physical states, Dirac observables and physical expectation values. Although restricted to special matter, it allows completion of the quantization program to the physical level and throws light on *how* a quantum singularity resolution may be viewed. For this reason, we this case is discussed in detail. Subsequently, Madhavan also showed another quantization for the same case, also completed to physical level, wherein holonomy corrections are absent and singularity resolution is achieved by inverse triad corrections only. There are also some issues which have been better understood in the past few years. These are briefly summarised and discussed in sections 4.2.2 and 4.2.3 .

4.1 FRW, Classical Theory

Classical model: Using coordinates adapted to the spatially homogeneous slicing of the space-time, the metric and the extrinsic curvature are given by,

$$ds^2 := -dt^2 + a^2(t) \{dr^2 + r^2 d\Omega^2\} \quad := \quad - dt^2 + a^2(t) ds_{\text{comoving}}^2 . \quad (4.1)$$

Starting from the usual Einstein-Hilbert action and scalar matter for definiteness, one can get to the Hamiltonian as,

$$\begin{aligned} S &:= \int dt \int_{\text{cell}} dx^3 \sqrt{|det g_{\mu\nu}|} \left\{ \frac{R(g)}{16\pi G} + \frac{1}{2} \dot{\phi}^2 - V(\phi) \right\} \\ &= V_0 \int dt \left\{ \frac{3}{8\pi G} (-a\dot{a}^2) + \frac{1}{2} a^3 \dot{\phi}^2 - V(\phi) a^3 \right\} \end{aligned} \quad (4.2)$$

$$p_a = -\frac{3V_0}{4\pi G} a\dot{a} \quad , \quad p_\phi = V_0 a^3 \dot{\phi} \quad , \quad V_0 := \int_{\text{cell}} d^3x \sqrt{g_{\text{comoving}}} ;$$

$$\begin{aligned} H(a, p_a, \phi, p_\phi) &= H_{\text{grav}} + H_{\text{matter}} \\ &= \left[-\frac{2\pi G}{3} \frac{p_a^2}{V_0 a} \right] + \left[\frac{1}{2} \frac{p_\phi^2}{a^3 V_0} + a^3 V_0 V(\phi) \right] \end{aligned} \quad (4.3)$$

$$= \left(\frac{3V_0 a^3}{8\pi G} \right) \left[-\frac{\dot{a}^2}{a^2} + \left(\frac{8\pi G}{3} \right) \left(\frac{H_{\text{matter}}}{V_0 a^3} \right) \right] \quad (4.4)$$

Thus, $H = 0 \leftrightarrow$ Friedmann Equation. For the spatially flat model, one has to choose a fiducial cell whose fiducial volume is denoted by V_0 .

In the connection formulation, instead of the metric one uses the densitized triad i.e. instead of the scale factor a one has $\tilde{p}, |\tilde{p}| := a^2$ while the connection variable is related to the extrinsic curvature as: $\tilde{c} := \gamma\dot{a}$ (the spin connections is absent for the flat model). Their Poisson bracket is given by $\{\tilde{c}, \tilde{p}\} = (8\pi G\gamma)/(3V_0)$. The arbitrary fiducial volume can be absorbed away by defining $c := V_0^{1/3}\tilde{c}$, $p := V_0^{2/3}\tilde{p}$. Here, γ is the Barbero-Immirzi parameter which is dimensionless and is determined from the Black hole entropy computations to be approximately 0.23 [8]. From now on we put $8\pi G := \kappa$. The classical Hamiltonian is then given by,

$$H = \left[-\frac{3}{\kappa} \left(\gamma^{-2} c^2 \sqrt{|p|} \right) \right] + \left[\frac{1}{2} |p|^{-3/2} p_\phi^2 + |p|^{3/2} V(\phi) \right] . \quad (4.5)$$

For future comparison, we now take the potential for the scalar field, $V(\phi)$ to be zero as well.

One can obtain the Hamilton's equations of motion and solve them easily. On the constrained surface ($H = 0$), eliminating c in favour of p and p_ϕ , one has,

$$\begin{aligned} c &= \pm \gamma \sqrt{\frac{\kappa}{6}} \frac{|p_\phi|}{|p|} \quad , \quad \dot{p} = \pm 2 \sqrt{\frac{\kappa}{6}} |p_\phi| |p|^{-1/2} . \\ \dot{\phi} &= p_\phi |p|^{-3/2} \quad , \quad \dot{p}_\phi = 0 , \end{aligned} \quad (4.6)$$

$$\frac{dp}{d\phi} = \pm \sqrt{\frac{2\kappa}{3}} |p| \quad \Rightarrow \quad \mathbf{p}(\phi) = \mathbf{p}_* \mathbf{e}^{\pm \sqrt{\frac{2\kappa}{3}}(\phi - \phi_*)} \quad (4.7)$$

Since ϕ is a monotonic function of the synchronous time t , it can be taken as a new ‘‘time’’ variable. The solution is determined by $p(\phi)$ which is (i) independent of the constant p_ϕ and (ii) passes through $p = 0$ as $\phi \rightarrow \pm\infty$ (expanding/contracting solutions). It is immediate that, along these curves, $p(\phi)$, the energy density ($p^{-6} p_\phi^2 / 2$) and the extrinsic curvature diverge as $p \rightarrow 0$. Furthermore, the divergence of the density implies that $\phi(t)$ is *incomplete* i.e. t ranges over a semi-infinite interval as ϕ ranges over the full real line¹.

¹For the FRW metric, integral curves of ∂_t are time-like geodesics and hence incompleteness with respect to t is synonymous with geodesic incompleteness.

Thus a singularity is signalled by *every* solution $p(\phi)$ passing through $p = 0$ in *finite* synchronous time (or equivalently by the density diverging somewhere along any solution). A natural way to ensure that *all* solutions are non-singular is to ensure that either of the two terms in the Hamiltonian constraint is *bounded*. Question is: *If and how does a quantum theory replace the Big Bang singularity by something non-singular?*

There are at least two ways to explore this question. One can imagine computing corrections to the Hamiltonian constraint such that individual terms in the effective constraint are bounded. This approach presupposes the classical framework and thus will have a *domain of validity of these corrections*. Alternatively and more satisfactorily, one should be able to define suitable Dirac observables whose expectation values will generate the analogue of $p(\phi)$ curves along which physical quantities such as energy density, remain bounded. Both are discussed below.

4.2 FRW, Quantum Theory

Schrodinger Quantization: In the standard Schrodinger quantization, one can introduce wave functions of p, ϕ and quantize the Hamiltonian operator by $c \rightarrow i\hbar\kappa\gamma/3\partial_p$, $p_\phi \rightarrow -i\hbar\partial_\phi$, in equation (4.5). With a choice of operator ordering, $\hat{H}\Psi(p, \phi) = 0$ leads to the Wheeler-De Witt partial differential equation which has singular coefficients. We will return to this later.

Loop Quantization: The background independent quantization of Loop Quantum Gravity however suggest a different quantization of the isotropic model. One should look for a Hilbert space on which only exponentials of c (holonomies of the connection) are well defined operators and not \hat{c} . Such a Hilbert space is obtained as the representation space of the C^* algebra of holonomies. In the present context this algebra is the algebra of *almost periodic functions of c* , finite linear combinations of functions of the form $e^{i\lambda_j c}$, $\lambda_j \in \mathbb{R}$. Inner product (analogue of the Ashtekar-Lewandowski measure) on the space of the almost periodic functions is given by:

$$(\Psi, \Phi) := \lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^T dc \Psi^*(c)\Phi(c) . \quad (4.8)$$

The single exponentials form an orthonormal set. Let us denote it as, $\langle c|\mu\rangle := \exp\{\frac{i}{2}\mu c\}$, $\mu \in \mathbb{R}$. The holonomy-flux representation can now be made explicit as:

$$\begin{aligned} \hat{p}|\mu\rangle &= \frac{1}{6}\gamma\ell_P^2\mu|\mu\rangle , \quad \langle\mu|\mu'\rangle = \delta_{\mu,\mu'} , \quad \mu \in \mathbb{R} \\ \widehat{h}_\nu|\mu\rangle &:= e^{\frac{i}{2}\nu c}|\mu\rangle = |\mu + \nu\rangle \end{aligned} \quad (4.9)$$

Notice that that the triad operator has every real number as a *proper eigenvalue* (i.e. has a corresponding *normalizable* eigenvector, the spectrum is *discrete*). This implies that the holonomy operator, is *not weakly continuous* in the label ν i.e. arbitrary matrix elements of \widehat{h}_ν are not continuous functions of ν . Therefore one *cannot* define a \hat{c} operator. Note that the *volume operator*, is given by $\hat{V} := |p|^{3/2}$.

Inverse Triad Operator: The fact that spectrum of the triad operator is *discrete*, has a major implication: *inverses of positive powers of triad operators do not exist*². These have

²The domain of the inverse power operator(s) will have to exclude the subspace corresponding to the zero eigenvalue of the triad operator. But this makes the domain *non-dense* and its adjoint cannot be defined [9].

to be defined by using alternative classical expressions and promoting them to quantum operators. This can be done with at least one parameter worth of freedom, eg.

$$|p|^{-1} = \left[\frac{3}{\kappa\gamma l} \{c, |p|^l\} \right]^{1/(1-l)}, \quad l \in (0, 1). \quad (4.10)$$

Only positive powers of $|p|$ appear now. However, this still cannot be used for quantization since there is no \hat{c} operator. One must use holonomies: $h_j(c) := e^{\mu_0 c \Lambda^i \tau_i}$, where τ_i are anti-hermitian generators of $SU(2)$ in the j^{th} representation satisfying $\text{Tr}_j(\tau_i \tau_j) = -\frac{1}{3}j(j+1)\delta_{ij}$, Λ^i is a unit vector specifying a direction in the Lie algebra of $SU(2)$ and μ_0 is the coordinate length of the edge used in defining the holonomy. It is a fraction of $V_0^{1/3}$. Using the holonomies,

$$|p|^{-1} = (8\pi G \mu_0 \gamma l)^{\frac{1}{1-l}} \left[\frac{3}{j(j+1)(2j+1)} \text{Tr}_j \Lambda \cdot \tau h_j \{h_j^{-1}, |p|^l\} \right]^{\frac{1}{1-l}}, \quad (4.11)$$

which can be promoted to an operator. Two parameters, $\mu_0 \in \mathbb{R}$ and $j \in \mathbb{N}/2$, have crept in and we have a three parameter family of inverse triad operators. The definitions are:

$$\widehat{|p|_{(j)l}^{-1}}|\mu\rangle = \left(\frac{2j\mu_0}{6} \gamma \ell_{\text{P}}^2 \right)^{-1} (F_l(q))^{\frac{1}{1-l}} |\mu\rangle, \quad q := \frac{\mu}{2\mu_0 j} := \frac{p}{2jp_0}, \quad (4.12)$$

$$F_l(q) := \frac{3}{2l} \left[\frac{1}{l+2} \{(q+1)^{l+2} - |q-1|^{l+2}\} - \frac{1}{l+1} q \{(q+1)^{l+1} - \text{sgn}(q-1)|q-1|^{l+1}\} \right]$$

$$F_l(q \gg 1) \approx [q^{-1}]^{1-l}, \quad (4.13)$$

$$F_l(q \approx 0) \approx \left[\frac{3q}{l+1} \right].$$

All these operators obviously commute with \hat{p} and their eigenvalues are bounded above. This implies that the matter densities (and also intrinsic curvatures for more general homogeneous models), remain bounded over the classically singular region. Most of the phenomenological novelties are consequences of this particular feature predominantly anchored in the matter sector. In the effective Hamiltonian computations, this modification will imply the second term in the Hamiltonian constraint (4.5) is rendered bounded implying singularity avoidance.

We have also introduced two scales: $p_0 := \frac{1}{6}\mu_0 \ell_{\text{P}}^2$ and $2jp_0 := \frac{1}{6}\mu_0 (2j) \ell_{\text{P}}^2$. The regime $|p| \ll p_0$ is termed the *deep quantum regime*, $p \gg 2jp_0$ is termed the *classical regime* and $p_0 \lesssim |p| \lesssim 2jp_0$ is termed the *semi-classical regime*. The modifications due to the inverse triad defined above are strong in the semi-classical and the deep quantum regimes. For $j = 1/2$ the semi-classical regime is absent. Note that such scales are not available for the Schrodinger quantization.

The Gravitational Constraint: Since \hat{c} operator does not exist, the gravitational Hamiltonian (the first bracket in eq.(4.5)), has to be expressed in an equivalent form using holonomies. For this, let us go back to the full theory Hamiltonian:

$$\frac{6}{\gamma^2} c^2 \sqrt{p} = \gamma^{-2} \int_{\text{cell}} d^3x \frac{\epsilon_{ijk} E^{ai} E^{bj} F_{ab}^k}{\sqrt{|\det E|}} \quad (4.14)$$

Now use the two identities:

$$\frac{\epsilon_{ijk} E^{ai} E^{bj}}{\sqrt{|\det E|}} = \sum_k \frac{4 \operatorname{sgn} p}{\kappa \gamma \mu_0 V_0^{1/3}} \epsilon^{abc} \omega_c^k \operatorname{Tr} \left(h_k^{(\mu_0)} \left\{ \left(h_k^{(\mu_0)} \right)^{-1}, V \right\} \tau_i \right) \quad (4.15)$$

$$F_{ab}^k = -2 \lim_{A_\square \rightarrow 0} \operatorname{Tr} \left(\frac{h_{\square ij}^{(\mu_0)} - 1}{\mu_0^2 V_0^{2/3}} \right) \tau^k \omega_a^i \omega_b^j \quad (4.16)$$

$$h_{\square ij}^{(\mu_0)} := h_i^{(\mu_0)} h_j^{(\mu_0)} \left(h_i^{(\mu_0)} \right)^{-1} \left(h_j^{(\mu_0)} \right)^{-1} \quad (4.17)$$

In the above, the fiducial cell is thought to have been sub-divided into smaller cells of side $\mu_0 \ell$, $\ell := V_0^{1/3}$. The area of a plaquette is $A_\square = \ell^2 \mu_0^2$. The plaquette is to be shrunk such that its area goes to zero. The superscript (μ_0) on the holonomies is to remind that the length of the edge is μ_0 . The 1-forms ω_a^i are the fiducial 1-forms whose square gives the fiducial metric and the ϵ^{abc} is the (fiducial) metric dependent Levi-Civita density.

In quantum geometry however there is a gap in the spectrum of area operator and thus it is *not* appropriate to take the area to zero, but at the most to the smallest possible eigenvalue. Independently, if we force the limit, it will imply $\mu_0 \rightarrow 0$ which in turn amounts to defining \hat{c} operator which does *not* exist on the Hilbert space.

Substituting these in the (4.14) and carrying out the integration over the cell leads to (suppressing the μ_0 superscript on the holonomies),

$$H_{\text{grav}} = -\frac{4}{8\pi G \gamma^3 \mu_0^3} \sum_{ijk} \epsilon^{ijk} \operatorname{Tr} \left(h_i h_j h_i^{-1} h_j^{-1} h_k \{ h_k^{-1}, V \} \right) \quad (4.18)$$

In the above, we have used $j = 1/2$ representation for the holonomies and V denotes the volume function. In the limit $\mu_0 \rightarrow 0$ one gets back the classical expression ³.

If we promote this expression to a quantum operator (modulo ordering ambiguities) on the LQC Hilbert space constructed above, then we *cannot* take the limit $\mu_0 \rightarrow 0$ because it would imply that \hat{c} exist which we have shown to be impossible. Thus, at the quantum level we should *not* take the limit $\mu_0 \rightarrow 0$. The best we can do is to take reduce μ_0 such that the area reaches its smallest possible (and non-zero due to the gap) eigenvalue $\Delta := (2\sqrt{3}\pi\gamma)\ell_P^2$. But which area do we consider, the fiducial or the physical? These are related by a factor of $|p|$. It seems appropriate to choose the physical area, which implies that we must take μ_0 to be a function $\bar{\mu}$ of p given by, $\bar{\mu}(p) := \sqrt{\Delta/|p|}$. Note that this is *one* prescription to interpret the limitation on shrinking of the plaquette. There are others which will be mentioned later. In the following we will continue to use the μ_0 notation and replace it by $\bar{\mu}(p)$ when needed.

While promoting this expression to operators, there is a choice of factor ordering involved and many are possible. We will present two choices of ordering: the *non-symmetric* one which keeps the holonomies on the left as used in the existing choice for the full theory, and the particular *symmetric* one used in [10].

$$\hat{H}_{\text{grav}}^{\text{non-sym}} = \frac{24i}{\gamma^3 \mu_0^3 \ell_P^2} \sin^2 \mu_0 c \left(\sin \frac{\mu_0 c}{2} \hat{V} \cos \frac{\mu_0 c}{2} - \cos \frac{\mu_0 c}{2} \hat{V} \sin \frac{\mu_0 c}{2} \right) \quad (4.19)$$

³The expression for the Hamiltonian constraint follows exactly from the full theory procedure. Starting from the equation (4.14), the integral will be replaced by a sum over smaller cells of a triangulation. The size parameter of the cells will drop out thanks to density weight 1 of the Hamiltonian. Due to homogeneity, contribution from each cell will be the same and hence the total sum will be number of cells of the triangulation times the contribution of one cell. There are exactly μ_0^{-3} cubical (say) cells with side of length $\mu_0 V_0^{1/3}$ and this produces the factor of μ_0^{-3} in equation (4.18). The V_0 of course disappears as in the full theory

$$\hat{H}_{\text{grav}}^{\text{sym}} = \frac{24i(\text{sgn}(p))}{\gamma^3 \mu_0^3 \ell_{\text{P}}^2} \sin \mu_0 c \left(\sin \frac{\mu_0 c}{2} \hat{V} \cos \frac{\mu_0 c}{2} - \cos \frac{\mu_0 c}{2} \hat{V} \sin \frac{\mu_0 c}{2} \right) \sin \mu_0 c \quad (4.20)$$

At the quantum level, μ_0 cannot be taken to zero since \hat{c} operator does not exist. The action of the Hamiltonian operators on $|\mu\rangle$ is obtained as,

$$\hat{H}_{\text{grav}}^{\text{non-sym}} |\mu\rangle = \frac{3}{\mu_0^3 \gamma^3 \ell_{\text{P}}^2} (V_{\mu+\mu_0} - V_{\mu-\mu_0}) (|\mu + 4\mu_0\rangle - 2|\mu\rangle + |\mu - 4\mu_0\rangle) \quad (4.21)$$

$$\begin{aligned} \hat{H}_{\text{grav}}^{\text{sym}} |\mu\rangle &= \frac{3}{\mu_0^3 \gamma^3 \ell_{\text{P}}^2} [|V_{\mu+3\mu_0} - V_{\mu+\mu_0}| |\mu + 4\mu_0\rangle + |V_{\mu-\mu_0} - V_{\mu-3\mu_0}| |\mu - 4\mu_0\rangle \\ &\quad - \{|V_{\mu+3\mu_0} - V_{\mu+\mu_0}| + |V_{\mu-\mu_0} - V_{\mu-3\mu_0}|\} |\mu\rangle] \end{aligned} \quad (4.22)$$

where $V_\mu := (\frac{1}{6}\gamma\ell_{\text{P}}^2|\mu|)^{3/2}$ denotes the eigenvalue of \hat{V} .

We also have the Hilbert space for the matter degrees which for us is a single scalar, ϕ and the full kinematical Hilbert space is the tensor product of the $L_2(\mathbb{R}_{\text{Bohr}}, d\mu_{\text{Bohr}}) \otimes \mathcal{H}_{\text{matter}}$.

Wheeler-DeWitt Difference Equation: Let $|\Psi\rangle := \sum_\mu \Psi(\mu, \phi) |\mu\rangle$, where the sum is over a countable subset of \mathbb{R} , the coefficients $\Psi(\mu, \phi)$ are valued in the matter Hilbert space and the argument ϕ is a reminder of that. The Hamiltonian constraint is imposed on these $|\Psi\rangle$ which leads to the *Wheeler-DeWitt equation* for the coefficients. Thanks to the presence of the trigonometric operators, this equation is a *difference equation*. In the Schrodinger quantization, this would be a differential equation.

For the non-symmetric operator we get,

$$\begin{aligned} A(\mu + 4\mu_0)\Psi(\mu + 4\mu_0, \phi) - 2A(\mu)\Psi(\mu, \phi) + A(\mu - 4\mu_0)\Psi(\mu - 4\mu_0, \phi) \\ = -\frac{2\kappa}{3}\mu_0^3\gamma^3\ell_{\text{P}}^2 H_{\text{matter}}(\mu)\Psi(\mu, \phi) \end{aligned} \quad (4.23)$$

where, $A(\mu) := V_{\mu+\mu_0} - V_{\mu-\mu_0}$ and vanishes for $\mu = 0$.

For the symmetric operator one gets,

$$\begin{aligned} f_+(\mu)\Psi(\mu + 4\mu_0, \phi) + f_0(\mu)\Psi(\mu, \phi) + f_-(\mu)\Psi(\mu - 4\mu_0, \phi) \\ = -\frac{2\kappa}{3}\mu_0^3\gamma^3\ell_{\text{P}}^2 H_{\text{matter}}(\mu)\Psi(\mu, \phi) \quad \text{where,} \end{aligned} \quad (4.24)$$

$$f_+(\mu) := |V_{\mu+3\mu_0} - V_{\mu+\mu_0}|, \quad f_-(\mu) := f_+(\mu - 4\mu_0), \quad f_0 := -f_+(\mu) - f_-(\mu).$$

Notice that $f_+(-2\mu_0) = 0 = f_-(-2\mu_0)$, but $f_0(\mu)$ is never zero. The absolute values have entered due to the $\text{sgn}(p)$ factor.

The difference equations relate $\Psi(\mu)$'s only for μ 's in a "lattice", $\mathcal{L}_{\hat{\mu}} := \{\mu = \hat{\mu} + 4\mu_0 n, n \in \mathbb{Z}\}$ and the coefficients labelled by different lattices are completely independent. The $\hat{\mu} \in [0, 4\mu_0)$, label different *superselected* sectors.

The equations are effectively second order difference equations and the $\Psi(\mu, \phi)$ are determined by specifying Ψ for two consecutive values of μ eg for $\mu = \hat{\mu} + 4\mu_0 N$ and $\mu = \hat{\mu} + 4\mu_0(N + 1)$. Since the highest (lowest) order coefficients vanishes for some μ , then the corresponding component $\Psi(\mu, \phi)$ is undetermined by the equation. Potentially this could introduce an arbitrariness in extending the Ψ specified by data in the classical regime (eg $\mu \gg 2j$) to the negative μ . Potentially, maintaining determinism of the quantum wave function, is one of the restrictive criteria for choosing the ordering.

For the non-symmetric case, the highest (lowest) A coefficients vanish for their argument equal to zero thus leaving the corresponding Ψ component undetermined. However, this undetermined component is decoupled from the others. Thus apart from admitting the trivial solution $\Psi(\mu, \phi) := \Phi(\phi)\delta_{\mu,0}$, $\forall \mu$, all other non-trivial solutions are completely determined by giving two consecutive components: $\Psi(\hat{\mu}, \phi)$, $\Psi(\hat{\mu} + 4\mu_0, \phi)$.

For the symmetric case, due to these properties of the $f_{\pm,0}(\mu)$, it looks as if the difference equation is *non-deterministic* if $\mu = 2\mu_0 + 4\mu_0 n$, $n \in \mathbb{Z}$. This is because for $\mu = -2\mu_0$, $\Psi(2\mu_0, \phi)$ is undetermined by the lower order Ψ 's and this coefficient enters in the determination of $\Psi(2\mu_0, \phi)$. However, the symmetric operator also commutes with the parity operator: $(\Pi\Psi)(\mu, \phi) := \Psi(-\mu, \phi)$. Consequently, $\Psi(2\mu_0, \phi)$ is determined by $\Psi(-2\mu_0, \phi)$. Thus, we can restrict to $\mu = 2\mu_0 + 4k\mu_0$, $k \geq 0$ where the equation *is* deterministic.

In both cases then, the space of solutions of the constraint equation, is completely determined by giving appropriate data for large $|\mu|$ i.e. in the classical regime. Such a deterministic nature of the constraint equation has been taken as a necessary condition for non-singularity at the quantum level ⁴.

Effective Hamiltonian: By introducing an interpolating, slowly varying smooth function, $\Psi(p(\mu) := \frac{1}{6}\gamma\ell_P^2\mu)$, and keeping only the first non-vanishing terms, one deduces the Wheeler-De Witt differential equation (with a modified matter Hamiltonian) from the above difference equation. Making a WKB approximation, one infers an effective Hamiltonian which matches with the classical Hamiltonian for large volume ($\mu \gg \mu_0$) and small extrinsic curvature (derivative of the WKB phase is small). There are terms of $o(\hbar^0)$ which contain arbitrary powers of the first derivative of the phase which can all be summed up. The resulting effective Hamiltonian now contains modifications of the classical gravitational Hamiltonian, apart from the modifications in the matter Hamiltonian due to the inverse powers of the triad. The largest possible domain of validity of effective Hamiltonian so deduced must have $|p| \gtrsim p_0$ [11, 12].

An effective Hamiltonian can alternatively be obtained by computing expectation values of the Hamiltonian operator in semi-classical states peaked in classical regimes [13]. The leading order effective Hamiltonian that one obtains is (spatially flat case):

$$\begin{aligned} H_{\text{eff}}^{\text{non-sym}} &= -\frac{1}{16\pi G} \left(\frac{6}{\mu_0^3 \gamma^3 \ell_P^2} \right) \left[B_+(p) \sin^2(\mu_0 c) + \left(A(p) - \frac{1}{2} B_+(p) \right) \right] + H_{\text{matter}} ; \\ B_+(p) &:= A(p + 4p_0) + A(p - 4p_0) , \quad A(p) := (|p + p_0|^{3/2} - |p - p_0|^{3/2}) , \\ p &:= \frac{1}{6} \gamma \ell_P^2 \mu , \quad p_0 := \frac{1}{6} \gamma \ell_P^2 \mu_0 . \end{aligned} \quad (4.25)$$

For the symmetric operator, the effective Hamiltonian is the same as above except that $B_+(p) \rightarrow f_+(p) + f_-(p)$ and $2A(p) \rightarrow f_+(p) + f_-(p)$.

The second bracket in the square bracket, is the quantum geometry potential which is negative and higher order in ℓ_P but is important in the small volume regime and plays a role in the genericness of bounce deduced from the effective Hamiltonian [14]. This term is absent in the effective Hamiltonian deduced from the symmetric constraint. The matter Hamiltonian

⁴For contrast, if one just symmetrizes the non-symmetric operator (without the sgn factor), one gets a difference equation which *is non-deterministic*. Note that this issue arises only in *one* superselection sector so may not really be an issue. However, requiring deterministic equation in *all* sectors could be invoked as a criterion to discriminate between different factor ordering.

will typically have the eigenvalues of powers of inverse triad operator which depend on the ambiguity parameters j, l .

We already see that the quantum modifications are such that both the matter (due to inverse volume corrections) and the gravitational part (due to holonomy corrections) in the effective Hamiltonian, are rendered bounded and effective dynamics must be non-singular.

For large values of the triad, $p \gg p_0$, $B_+(p) \sim 6p_0\sqrt{p} - o(p^{-3/2})$ while $A(p) \sim 3p_0\sqrt{p} - o(p^{-3/2})$. In this regime, the effective Hamiltonians deduced from both symmetric and non-symmetric ordering are the same⁵. The classical Hamiltonian is obtained for $\mu_0 \rightarrow 0$. From this, one can obtain the equations of motion and by computing the left hand side of the Friedmann equation, infer the effective energy density. For $p \gg p_0$ one obtains⁶,

$$\frac{3}{8\pi G} \left(\frac{\dot{a}^2}{a^2} \right) := \rho_{\text{eff}} = \left(\frac{H_{\text{matter}}}{p^{3/2}} \right) \left\{ 1 - \frac{8\pi G \mu_0^2 \gamma^2}{3} p \left(\frac{H_{\text{matter}}}{p^{3/2}} \right) \right\}, \quad p := a^2/4. \quad (4.26)$$

The effective density is quadratic in the classical density, $\rho_{cl} := H_{\text{matter}} p^{-3/2}$. This modification is due to the quantum correction in the gravitational Hamiltonian (due to the \sin^2 feature). This is over and above the corrections hidden in the matter Hamiltonian (due to the “inverse volume” modifications). As noted before, we have two scales: p_0 controlled by μ_0 in the gravitational part and $2p_0j$ in the matter part. For large j it is possible that we can have $p_0 \ll p \ll 2p_0j$ in which case the above expressions will hold with j dependent corrections in the matter Hamiltonian. In this semi-classical regime, the corrections from \sin^2 term are smaller in comparison to those from inverse volume. If $p \gg 2p_0j$ then the matter Hamiltonian is also the classical expression. For $j = 1/2$, there is only the $p \gg p_0$ regime and ρ_{cl} is genuinely the classical density.

To summarize:

(1) The connection formulation, in the homogeneous and isotropic context, uses variables $(c, p \in \mathbb{R})$ in terms of which the classical singularity ($p = 0$) is in the *interior* of the phase space. By contrast, in the ADM variables $(a \geq 0, K)$, in the same context, the classical singularity ($a = 0$) is on the *boundary*. This requires a boundary condition on the quantum wave functions to be specified in the deep quantum region where the classical framework is suspect. When the singularity is in the interior, only a continuation of the quantum wave function is required, given its specification in the semi-classical region.

(2) The connection variables also strongly motivate the very different *loop quantization*. Its immediate implications are two types of corrections - the holonomy corrections and the inverse triad corrections. *Either* of these is sufficient to indicate a bounce in the effective Hamiltonian picture. The same use of holonomies make the Wheeler-DeWitt equation, a *difference equation*.

(3) The analysis at the level of effective Hamiltonian already indicates (i) replacement of big bang by big bounce; (ii) natural prediction of an inflationary (accelerated) phase; (iii) singularity resolution for more general homogeneous models with curvature.

⁵The effective Hamiltonian then reduces to $-\frac{3}{\kappa} \gamma^{-2} \sqrt{p} [\mu_0^{-2} \sin^2(\mu_0 c)]$. This is also the Hamiltonian in eq. (4.18) for non-zero μ_0 .

⁶For p in the semi-classical regime, one should include the contribution of the quantum geometry potential present in the non-symmetric ordering, especially for examining the bounce possibility [12].

(4) There are at least three distinct ambiguity parameters: μ_0 related to the fiducial length of the loop used in writing the holonomies; j entering in the choice of $SU(2)$ representation which is chosen to be $1/2$ in the gravitational sector and some large value in the matter sector; l entering in writing the inverse powers in terms of Poisson brackets. The first one was thought to be determined by the area gap from the full theory. The $j = 1/2$ in the gravitational Hamiltonian seems needed to avoid high order difference equation and larger j values are hinted to be problematic in the study of a three dimensional model [15]. Given this, the choice of a high value of j in the matter Hamiltonian seems unnatural⁷. Nevertheless the higher values of j in the matter sector allow for a larger semi-classical regime. The l does not play as significant a role.

(5) LQC being a constrained theory, it would be more appropriate if singularity resolution is formulated and demonstrated in terms of physical expectation values of physical (Dirac) operators i.e. in terms of “gauge invariant quantities”. This can be done at present with self-adjoint constraint i.e. a symmetric ordering and for free, massless scalar matter.

Physical quantities and Singularity Resolution: When the Hamiltonian is a constraint, at the classical level itself, the notion of dynamics in terms of the ‘time translations’ generated by the Hamiltonian is devoid of any *physical* meaning. Furthermore, at the quantum level when one attempts to impose the constraint as $\hat{H}|\Psi\rangle = 0$, typically one finds that there are no solutions in the Hilbert space on which \hat{H} is defined - the solutions are generically distributional. One then has to consider the space of all distributional solutions, define a new physical inner product to turn it into a Hilbert space (the physical Hilbert space), define operators on the space of solutions (which must thus act invariantly) which are self-adjoint (physical operators) and compute expectation values, uncertainties etc of these operators to make physical predictions. Clearly, the space of solutions depends on the quantization of the constraint and there is an arbitrariness in the choice of physical inner product. This is usually chosen so that a complete set of Dirac observables (as deduced from the classical theory) are self-adjoint. This is greatly simplified if the constraint has a *separable* form with respect to some degree of freedom⁸. For LQC (and also for the Wheeler-De Witt quantum cosmology), such a simplification is available for a free, massless scalar matter: $H_{\text{matter}}(\phi, p_\phi) := \frac{1}{2}p_\phi^2|p|^{-3/2}$. Let us sketch the steps schematically, focusing on the spatially flat model for simplicity [10, 17].

1. *Fundamental constraint equation:*

The classical constraint equations is:

$$-\frac{6}{\gamma^2}c^2\sqrt{|p|} + 8\pi G p_\phi^2 |p|^{-3/2} = 0 = C_{\text{grav}} + C_{\text{matter}} ; \quad (4.27)$$

The corresponding quantum equation for the wave function, $\Psi(p, \phi)$ is:

$$8\pi G \hat{p}_\phi^2 \Psi(p, \phi) = [\tilde{B}(p)]^{-1} \hat{C}_{\text{grav}} \Psi(p, \phi) , \quad [\tilde{B}(p)] \text{ is eigenvalue of } \widehat{|p|^{-3/2}} ; \quad (4.28)$$

Putting $\hat{p}_\phi = -i\hbar\partial_\phi$, $p := \frac{\gamma\ell_P^2}{6}\mu$ and $\tilde{B}(p) := (\frac{\gamma\ell_P^2}{6})^{-3/2}B(\mu)$, the equation can be written in a separated form as ⁹,

$$\frac{\partial^2 \Psi(\mu, \phi)}{\partial \phi^2} = [B(\mu)]^{-1} \left[8\pi G \left(\frac{\gamma}{6}\right)^{3/2} \ell_P^{-1} \hat{C}_{\text{grav}} \right] \Psi(\mu, \phi) := -\hat{\Theta}(\mu)\Psi(\mu, \phi). \quad (4.29)$$

⁷For an alternative view on using large values of j , see reference [16].

⁸A general abstract procedure using group averaging is also available.

⁹Our primary goal here is to compare the classical geometry (Wheeler-DeWitt quantization) and quantum

The $\hat{\Theta}$ operator for different quantizations is different. For Schrodinger quantization (Wheeler-De Witt), with a particular factor ordering suggested by the continuum limit of the difference equation, the operator $\hat{\Theta}(\mu)$ is given by,

$$\hat{\Theta}_{\text{Sch}}(\mu)\Psi(\mu, \phi) = -\frac{16\pi G}{3}|\mu|^{3/2}\partial_\mu(\sqrt{\mu}\partial_\mu\Psi(\mu, \phi)) \quad (4.30)$$

while for LQC, with symmetric ordering, it is given by,

$$\begin{aligned} \hat{\Theta}_{\text{LQC}}(\mu)\Psi(\mu, \phi) &= -[B(\mu)]^{-1} \{ C^+(\mu)\Psi(\mu + 4\mu_0, \phi) + C^0(\mu)\Psi(\mu, \phi) + \\ &\quad C^-(\mu)\Psi(\mu - 4\mu_0, \phi) \} , \\ C^+(\mu) &:= \frac{\pi G}{9\mu_0^3} | |\mu + 3\mu_0|^{3/2} - |\mu + \mu_0|^{3/2} | , \\ C^-(\mu) &:= C^+(\mu - 4\mu_0) , \quad C^0(\mu) := -C^+(\mu) - C^-(\mu) . \end{aligned} \quad (4.31)$$

Note that in the Schrodinger quantization, the $B_{\text{Sch}}(\mu) = |\mu|^{-3/2}$ diverges at $\mu = 0$ while in LQC, $B_{\text{LQC}}(\mu)$ vanishes for all allowed choices of ambiguity parameters. In both cases, $B(\mu) \sim |\mu|^{-3/2}$ as $|\mu| \rightarrow \infty$.

2. Inner product and General solution:

The operator $\hat{\Theta}$ turns out to be a self-adjoint, positive definite operator on the space of functions $\Psi(\mu, \phi)$ for each fixed ϕ with an inner product scaled by $B(\mu)$. That is, for the Schrodinger quantization, it is an operator on $L^2(\mathbb{R}, B_{\text{Sch}}(\mu)d\mu)$ while for LQC it is an operator on $L^2(\mathbb{R}_{\text{Bohr}}, B_{\text{Bohr}}(\mu)d\mu_{\text{Bohr}})$. Because of this, the operator has a complete set of eigenvectors¹⁰:

$$\hat{\Theta}e_k(\mu) = \omega^2(k)e_k(\mu) , \quad \langle e_k | e_{k'} \rangle = \delta(k, k') , \quad k, k' \in \mathbb{R}. \quad (4.32)$$

Consequently, the general solution of the fundamental constraint equation can be expressed as

$$\Psi(\mu, \phi) = \int dk \tilde{\Psi}_+(k)e_k(\mu)e^{i\omega(k)\phi} + \tilde{\Psi}_-(k)\bar{e}_k(\mu)e^{-i\omega(k)\phi} . \quad (4.33)$$

The orthonormality relations among the $e_k(\mu)$ are in the corresponding Hilbert spaces. Different quantizations differ in the form of the eigenfunctions, possibly the spectrum itself and of course $\omega(k)$. In general, these solutions are *not* normalizable in $L^2(\mathbb{R}_{\text{Bohr}} \times \mathbb{R}, B_{\text{Bohr}}(\mu)d\mu_{\text{Bohr}} \times d\mu)$, i.e. these are distributional.

Remarks:

(1) The $\hat{\Theta}$ operator acts in each of the superselected sector (thanks to the difference equation structure) and these are *separable*. Hence Dirac- δ appears in general when the label takes *continuous* values.

(2) The group averaging can be seen as follows. Given any $f(\mu, \phi)$ one defines its *group average*,

$$\Psi_f(\mu, \phi) := \int_{-\infty}^{\infty} d\lambda e^{i\lambda\hat{C}_{\text{tot}}} f(\mu, \phi) ; \quad \hat{C}_{\text{tot}} := \frac{\partial^2}{\partial\phi^2} + \hat{\Theta} ,$$

geometry (loop quantization). Consequently, the gravitational constraint is quantized in two different ways but for *simplicity*, the matter sector is quantized in the usual Schrodinger way. In both quantizations, $p_\phi = -i\hbar\partial_\phi$ and there is no ϕ dependence in the matter Hamiltonian, so the two quantum Hamiltonian will have identical expressions. However, using ϕ as labelling an ‘emergent time’ would be questionable.

¹⁰For the Schrodinger quantization, the explicit eigenfunctions are: $e_k(\mu) := \frac{|\mu|^{1/4}}{4\pi} e^{ik\ell n|\mu|}$ and the eigenvalues are: $\omega^2(k) := \frac{2\kappa}{3}(k^2 + 1/16)$ [17].

The eigenfunctions of the constraint operator are of a product form thanks to separability,

$$\frac{\partial^2}{\partial \phi^2} g_\sigma(\phi) = -\sigma^2 g_\sigma(\phi) \quad , \quad \hat{\Theta} e_k(\mu) = \omega^2(k) e_k(\mu) \quad , \quad g_\sigma(\phi) = e^{i\sigma\phi} \quad , \quad k, \sigma \in \mathbb{R}$$

Expanding the general function $f(\mu, \phi)$ in the eigenbasis of the constraint operator,

$$f(\mu, \phi) := \int dk \int d\sigma A_{k,\sigma} g_\sigma(\phi) e_k(\mu) \quad ,$$

implies,

$$\begin{aligned} \Psi_f(\mu, \phi) &= \int dk \int d\sigma A_{k,\sigma} g_\sigma(\phi) e_k(\mu) \delta(\sigma^2 - \omega^2(k)) \\ &= \int_{-\infty}^{\infty} \frac{dk}{2|\omega(k)|} [\{A_{k,\omega(k)} e^{i\omega(k)\phi} + A_{k,-\omega(k)} e^{-i\omega(k)\phi}\} e_\omega(\mu)] \end{aligned} \quad (4.34)$$

In the second equation above, we have carried out the integration over σ using $\delta(\sigma^2 - \omega^2(k)) = \frac{1}{2|\omega(k)|} (\delta(\sigma - \omega(k)) + \delta(\sigma + \omega(k)))$. Clearly the group average of a general function reproduces precisely the general solution given in equation (4.33).

3. Choice of Dirac observables:

Since the classical kinematical phase space is 4 dimensional and we have a single first class constraint, the phase space of physical states (reduced phase space) is two dimensional and we need two functions to coordinatize this space. We should thus look for two (classical) Dirac observables: functions on the kinematical phase space whose Poisson bracket with the Hamiltonian constraint vanishes on the constraint surface. Specific values of these functions serve to label the physics states. Thus physical observables are values of the Dirac observables. Classically, the Dirac observables can be obtained as follows.

Our constraint is: $p_\phi^2/2 - \frac{3}{\kappa} \gamma^{-2} c^2 p^2 \simeq 0$. A Dirac observable is a function $f(\phi, p_\phi, c, p)$ whose Poisson bracket with the constraint vanishes on the constraint surface. We can describe the constraint surface by solving for c as: $c(\phi, p_\phi, p) := \pm \sqrt{\kappa/6} \gamma p_\phi p^{-1}$ (say). Consequently it should suffice to consider the Dirac observables to be a function of (ϕ, p_ϕ, p) (we need only two independent Dirac observables). Then the Dirac observables are defined by the differential equation,

$$\frac{\partial f}{\partial \phi} \pm \sqrt{2\kappa/3} \frac{\partial f}{\partial \ln p} = 0 \quad \Rightarrow \quad f = f(\zeta, p_\phi) \quad , \quad \zeta := \phi \mp \sqrt{\frac{3}{2\kappa}} \ln p \quad .$$

Evidently, $f = p_\phi$ is a Dirac observable. For the second one, we can choose any function of ζ . A particularly convenient choice is: $f(\zeta(\phi, p)) := \# \exp\{\mp \sqrt{2\kappa/3} \zeta\} = p \exp\{\mp \sqrt{2\kappa/3} (\phi - \phi_0)\}$. These Dirac observables taking a particular value, say p_* , define curves in the (p, ϕ) plane, $p(\phi) := p_* \exp\{\pm \sqrt{2\kappa/3} (\phi - \phi_0)\}$ which are the classical solutions in (4.7).

In the quantum theory, the notion of Dirac observable is that it is an operator which maps solutions of the constraint to (other) solutions. We already have the general solution in eq (4.33) which is obtained via unitary evolution (in ϕ) from an initial $\Psi_\pm(\phi_0, \mu)$. Hence a Dirac observable is constructed by defining an operator on

$\Psi_{\pm}(\phi_0, \mu)$ to generate a new ‘initial state’, and evolving the new state by the unitary operator, thereby constructing a new solution of the constraint. This procedure is followed for the two Dirac operators corresponding to $f_1(\phi, p_\phi, p) := p_\phi$ and $f_2(\phi, p_\phi, p) := p \exp\{\mp\sqrt{2\kappa/3}(\phi - \phi_0)\}$. Notice that at $\phi = \phi_0$, these become the functions: p_ϕ and p respectively and they act on the wavefunctions as the differential operator $-i\hbar\partial_\phi$ and as the multiplicative operator p , respectively. Explicit construction is as follows.

Consider initial data, $\Psi_{\pm}(\mu, \phi_0)$, with the corresponding solution is denoted by,

$$\Psi(\mu, \phi) := e^{i\sqrt{\hat{\Theta}}(\phi-\phi_0)}\Psi_+(\mu, \phi_0) + e^{-i\sqrt{\hat{\Theta}}(\phi-\phi_0)}\Psi_-(\mu, \phi_0) .$$

Generate *new initial data* via the actions of $\hat{p}_\phi, |\widehat{\mu}|_{\phi_0}$ as,

$$|\widehat{\mu}|_{\phi_0}\Psi_{\pm}(\mu, \phi_0) := |\mu|\Psi_{\pm}(\mu, \phi_0) , \quad \hat{p}_\phi\Psi_{\pm}(\mu, \phi_0) := \hbar\sqrt{\hat{\Theta}}\Psi_{\pm}(\mu, \phi_0) . \quad (4.35)$$

Evolve these respectively, by $e^{\pm i\sqrt{\hat{\Theta}}(\phi-\phi_0)}$. By construction, these are solutions of the constraints, being of the form of (4.33). Explicitly,

$$\begin{aligned} \hat{p}_\phi\Psi(\mu, \phi) &:= e^{i\sqrt{\hat{\Theta}}(\phi-\phi_0)}(\hbar\sqrt{\hat{\Theta}})\Psi_+(\mu, \phi_0) + e^{-i\sqrt{\hat{\Theta}}(\phi-\phi_0)}(-\hbar\sqrt{\hat{\Theta}})\Psi_-(\mu, \phi_0) \\ &= -i\hbar\partial_\phi\Psi(\mu, \phi) , \end{aligned} \quad (4.36)$$

$$|\widehat{\mu}|_{\phi_0}\Psi(\mu, \phi) := e^{i\sqrt{\hat{\Theta}}(\phi-\phi_0)}|\mu|\Psi_+(\mu, \phi_0) + e^{-i\sqrt{\hat{\Theta}}(\phi-\phi_0)}|\mu|\Psi_-(\mu, \phi_0) \quad (4.37)$$

Expectation values and uncertainties of these operators are used to track the quantum ‘evolution’.

4. *Physical inner product:*

It follows that the Dirac operators defined on the space of solutions are self-adjoint if we define a *physical inner product* on the space of solutions as:

$$\langle\Psi|\Psi'\rangle_{\text{phys}} := \text{“} \int_{\phi=\phi_0} d\mu B(\mu)\text{”} \bar{\Psi}(\mu, \phi)\Psi'(\mu, \phi) . \quad (4.38)$$

Thus the eigenvalues of the inverse volume operator crucially enter the definition of the physical inner product. For Schrodinger quantization, the integral is really an integral while for LQC it is actually a sum over μ taking values in a lattice. The inner product is independent of the choice of ϕ_0 .

A complete set of physical operators and physical inner product has now been specified and physical questions can be phrased in terms of (physical) expectation values of functions of these operators.

5. *Semi-classical states:*

To discuss semi-classical regime, typically one *defines* semi-classical states: physical states such that a chosen set of self-adjoint operators have specified expectation values with uncertainties bounded by specified tolerances. A natural choice of operators for us are the two Dirac operators defined above.

To be definite, let us consider the Wheeler-De Witt quantization. An arbitrary wavefunction at some given ϕ_0 is expressed as an integral over k of the eigenfunctions $e_k(\mu)$

multiplied by some function of k and by a phase factor $e^{i\omega(k)\phi_0}$. The inner product involves integral over μ . We can arrange to have a peak at some particular value $|\mu_*|$ by introducing a factor of $-\sqrt{3/2\kappa}|\mu_*|$ so that for large k , the μ -integral will be dominated by $\mu \sim \mu_*$. A large value of k can be picked-up by choosing the function of k to be a suitable Gaussian. This particular large value can be related to a desired p_ϕ^* . Here are the expressions:

$$\Psi_{\text{semi}}(\mu, \phi_0) := \int dk e^{-\frac{(k-k^*)^2}{2\sigma^2}} e_k(\mu) e^{i\omega(\phi_0-\phi^*)} \quad (4.39)$$

$$k^* = -\sqrt{3/2\kappa}\hbar^{-1}p_\phi^* , \quad \phi^* = \phi_0 - \sqrt{3/2\kappa}\ell n|\mu_*| . \quad (4.40)$$

The Gaussian allows the integrand to be approximated by

$$e_{k^*}(\mu) e^{i\omega(k^*)(\phi_0-\phi^*)} \sim e^{i\ell n|\mu|k^* + i(\omega(k^*)\sqrt{3/2\kappa}\ell n|\mu_*|)} \sim e^{ik^*\ell n|\mu/\mu_*|}$$

where, in the last equality we used: k^* is large and $\omega(k^*) \simeq -\sqrt{2\kappa/3} k^*$ (see the footnote 10). The integral in the inner product will now pick-up contribution from near $\mu \simeq \mu_*$. With these observations, it is easy to verify that the ‘initial’ semiclassical wave function given above gives $\langle \hat{p}_\phi \rangle = p_\phi^*$ and $\langle \widehat{|\mu|_{\phi_0}} \rangle = \mu_*$. The initial semiclassical wavefunction evolves into $\Psi_{\text{semi}}(\mu, \phi)$ which is same as the initial wave function with $\phi_0 \rightarrow \phi$ ¹¹.

For LQC, the $e_k(\mu)$ functions are different [17] and the physical expectation values are to be evaluated using the physical inner product defined in the LQC context.

6. Evolution of physical quantities:

We have now the physical wave function, evolved from Ψ_{semi} . Since it retains the form of the initial wavefunction, the k integral can be approximated as before and thus will lead to same expectation value for \hat{p}_ϕ for all ϕ . For the expectation value of $\langle \widehat{|\mu|_{\phi_0}} \rangle(\phi)$, the μ integral will be saturated by the new phase, $\phi - \phi_0 + \sqrt{3/2\kappa} \ell n|\mu/\mu_*| \simeq 0$. And this we recognize as precisely the solution (4.7).

Thus, in the WdW quantization, the classical relational evolution, $p = p(\phi)$ is reproduced by the expectation values of the Dirac observables.

Exercise: compute/estimate the uncertainties of the Dirac observables in the semiclassical state given above..

7. Resolution of Big Bang Singularity:

A classical solution is obtained as a curve in (μ, ϕ) plane, different curves being labelled by the points (μ^*, ϕ^*) in the plane. The curves are independent of the constant value of p_ϕ^* . These curves are already given in (4.7).

Quantum mechanically, we first select a semi-classical solution, $\Psi_{\text{semi}}(p_\phi^*, \mu^* : \phi)$ in which the expectation values of the Dirac operators, at $\phi = \phi_0$, are p_ϕ^* and μ^* respectively. These values serve as labels for the semi-classical solution. The former one continues to be p_ϕ^* for all ϕ whereas $\langle \widehat{|\mu|_{\phi_0}} \rangle(\phi) =: |\mu|_{p_\phi^*, \mu^*}(\phi)$, determines a curve in the

¹¹In the above heuristic reasoning for the form of the semiclassical state, we have glossed over some technical issues such as whether the states exhibited are in the domain of the $\hat{\Theta}$ operator which requires carefully stipulating conditions on the function of k (which has been taken to be a Gaussian). These are too technical to go into here and are not expected to affect the corresponding discussion for LQC. A discussion of these issues may be seen in [18].

(μ, ϕ) plane. (We determined this curve above, using stationarity of the phase for the Schrodinger quantization). In general one expects this curve to be different from the classical curve in the region of small μ (small volume). This is what happens for the loop quantized theory.

The result of the computations is that Schrodinger quantization, the curve $|\mu|_{p_\phi^*, \mu^*}(\phi)$, does approach the $\mu = 0$ axis asymptotically. However for LQC, the curve *bounces away* from the $\mu = 0$ axis. In this sense – and now inferred in terms of physical quantities – the Big Bang singularity is resolved in LQC. It also turns out that for large enough values of p_ϕ^* , the quantum trajectories constructed by the above procedure are well approximated by the trajectories by the effective Hamiltonian. All these statements are for semi-classical solutions which are peaked at large μ_* at late times.

Two further features are noteworthy as they corroborate the suggestions from the effective Hamiltonian analysis.

First one is revealed by computing expectation value of the matter density operator, $\rho_{\text{matter}} := \frac{1}{2}(p_\phi^*)^2|p|^{-3}$, at the bounce value of $|p|$. It turns out that this value is sensitive to the value of p_ϕ^* and can be made arbitrarily *small* by choosing p_ϕ^* to be *large*. Physically this is unsatisfactory as quantum effects are *not* expected to be significant for matter density very small compared to the Planck density. This is traced to the quantization of the gravitational Hamiltonian, in particular to the step which introduces the ambiguity parameter μ_0 . A novel solution proposed in the “improved quantization”, removes this undesirable feature.

The second one refers to the role of quantum modifications in the gravitational Hamiltonian compared to those in the matter Hamiltonian (the inverse volume modification or $B(\mu)$). The former is much more significant than the latter. So much so, that even if one uses the $B(\mu)$ from the Schrodinger quantization (i.e. switch-off the inverse volume modifications), one still obtains the bounce. So bounce is seen as the consequence of $\hat{\Theta}$ being different and as far as qualitative singularity resolution is concerned, the inverse volume modifications are *un-important*. As the effective picture (for symmetric constraint) showed, the bounce occurs in the classical region (for $j = 1/2$) where the inverse volume corrections can be neglected. For an exact model which seeks to understand why the bounces are seen, please see [19].

Improved Quantization: The undesirable features of the bounce coming from the classical region, can be seen readily using the effective Hamiltonian, as remarked earlier. To see the effects of modifications from the gravitational Hamiltonian, choose $j = 1/2$ and consider the Friedmann equation derived from the effective Hamiltonian leading to the effective energy density (4.26), with matter Hamiltonian given by $H_{\text{matter}} = \frac{1}{2}p_\phi^2|p|^{-3/2}$. The positivity of the effective density implies that $p \geq p_*$ with p_* determined by vanishing of the effective energy density: $\rho_* := \rho_{cl}(p_*) = (\frac{8\pi G\mu_0^2\gamma^2}{3}p_*)^{-1}$. This leads to $|p_*| = \sqrt{\frac{4\pi G\mu_0^2\gamma^2}{3}}|p_\phi|$ and $\rho_* = \sqrt{2}(\frac{8\pi G\mu_0^2\gamma^2}{3})^{-3/2}|p_\phi|^{-1}$. One sees that for large $|p_\phi|$, the bounce scale $|p_*|$ can be large and the maximum density – density at bounce – could be small. Thus, *within the model*, there exist a possibility of seeing quantum effects (bounce) even when neither the energy density nor the bounce scale are comparable to the corresponding Planck quantities and this is an undesirable feature of the model. This feature is independent of factor ordering as long as the bounce occurs in the classical regime.

One may notice that *if* we replace $\mu_0 \rightarrow \bar{\mu}(p) := \sqrt{\Delta/|p|}$ where Δ is a constant, then the effective density vanishes when ρ_{cl} equals the critical value $\rho_{\text{crit}} := (\frac{8\pi G\Delta\gamma^2}{3})^{-1}$, which is

independent of matter Hamiltonian. The bounce scale p_* is determined by $\rho_* = \rho_{\text{crit}}$ which gives $|p_*| = (\frac{p_\phi^2}{2\rho_{\text{crit}}})^{1/3}$. Now although the bounce scale can again be large depending upon p_ϕ , the density at bounce is always the universal value determined by Δ . This is a rather nice feature in that quantum geometry effects are revealed when matter density (which couples to gravity) reaches a universal, critical value regardless of the dynamical variables describing matter. For a suitable choice of Δ one can ensure that a bounce always happens when *the energy density* becomes comparable to the Planck density. In this manner, one can retain the good feature (bounce) even for $j = 1/2$ thus “effectively fixing” an ambiguity parameter and also trade another ambiguity parameter μ_0 for Δ . This is precisely what is achieved by the “improved quantization” of the gravitational Hamiltonian [20].

The place where the quantization procedure is modified is when one expresses the curvature in terms of the holonomies along a loop around a “plaquette”. One shrinks the plaquette in the limiting procedure. One now makes an important departure: the plaquette should be shrunk only till the physical area (as distinct from a fiducial one) reaches its minimum possible value which is given by the area gap in the known spectrum of area operator in quantum geometry: $\Delta = 2\sqrt{3}\pi\gamma G\hbar$. Since the plaquette is a square of fiducial length μ_0 , its physical area is $\mu_0^2|p|$ and this should set be to Δ . Since $|p|$ is a dynamical variable, μ_0 cannot be a constant and is to be thought of a function on the phase space, $\bar{\mu}(p) := \sqrt{\Delta/|p|}$. Thus we need to define an operator corresponding to the classical expression: $h_f := \exp(i\frac{1}{2}f(p)c)$, we have taken a general function $f(p)$. This is little non-trivial since there is no \hat{c} operator and c, p are conjugate variables.

Observe that the usual holonomy operator effects a shift in the argument of eigenstates of the triad operator and formally the operator looks like $\exp(\nu\frac{d}{d\mu})$ i.e. it effects the action of a *finite* diffeomorphism generated by a vector field on the wavefunction. We will take this as a guiding principle.

Let Φ_f denote a diffeomorphism effecting a *unit parameter shift* along the integral curve of the vector field $f(\mu)\frac{d}{d\mu}$ and Φ_f^* , the corresponding pull-back map. We define $\widehat{h}_f\Psi(\mu) := [\Phi_f^*(\Psi)] := \Psi(\Phi_f(\mu))$. As argued above, for a constant function, this reduces to the usual action (4.9). It can be checked directly that this action is also *unitary* in the kinematical Hilbert space: $(\Phi, \Psi) = \sum_\mu \Phi^*(\mu)\Psi(\mu)$ where the sum is over a countable set (this follows from $|\Psi\rangle := \sum_{\mu \in \text{countable subset} \subset \mathbb{R}} \Psi(\mu)|\mu\rangle$)¹².

To compute a unit parameter shift due to the diffeomorphism generated by $f(\mu)$, solve the equation

$$\int_\mu^{\mu'} \frac{dx}{f(x)} = \int_v^{v+1} dv = 1 \quad (4.41)$$

This will give $\mu' := \Phi_f(\mu)$.

For the specific choice of $f(p) := \bar{\mu}(p) := \sqrt{\Delta}|p|^{-1/2}$, $\Delta := \gamma\sqrt{3}\ell_P^2/4$, $p(\mu) = \gamma\ell_P^2\mu/6$, one gets,

$$\begin{aligned} \sqrt{\frac{\Delta}{|p|}} &= \sqrt{\frac{3\sqrt{3}}{2}}|\mu|^{-1/2} =: f(\mu) && \Rightarrow \\ \text{sgn}(\mu')|\mu'|^{3/2} &= \text{sgn}(\mu)|\mu|^{3/2} + K^{-1} && K := \frac{2}{3}\sqrt{\frac{2}{3\sqrt{3}}} \end{aligned} \quad (4.42)$$

¹²For a comparison in Schrodinger quantization, see remarks in [17].

$$\left[\widehat{e^{f(\mu) \frac{d}{d\mu}} \Psi} \right] (\mu) := \Psi(\mu').$$

It is evident from the above that if we define $v := K \text{sgn}(\mu) |\mu|^{3/2}$, then the middle eqn reads: $v' = v + 1$. This suggests that we use $|v\rangle$ as a basis instead of $|\mu\rangle$. Apart from the constant K , and the sgn , v is related to the eigenvalue of the volume operator $|p|^{3/2}$. Note that v as a function of μ is one-to-one and on-to. Using the $h_{\bar{\mu}}$ operator and a basis labelled by volume eigenvalues, the Hamiltonian constraint is defined and difference equation is obtained as before. The relevant expressions are:

$$v := K \text{sgn}(\mu) |\mu|^{3/2} ; \quad (4.43)$$

$$\hat{V}|v\rangle = \left(\frac{\gamma}{6}\right)^{3/2} \frac{\ell_{\text{P}}^3}{K} |v| |v\rangle , \quad (4.44)$$

$$\widehat{e^{ik \frac{\bar{\mu}}{2} c}} \Psi(v) := \Psi(v+k) , \quad (4.45)$$

$$\widehat{|p|^{-1/2}} \Big|_{j=1/2, l=3/4} \Psi(v) = \frac{3}{2} \left(\frac{\gamma \ell_{\text{P}}^2}{6}\right)^{-1/2} K^{1/3} |v|^{1/3} \left| |v+1|^{1/3} - |v-1|^{1/3} \right| \Psi(v) \quad (4.46)$$

$$B(v) = \left(\frac{3}{2}\right)^{3/2} K |v| \left| |v+1|^{1/3} - |v-1|^{1/3} \right|^3 \quad (4.47)$$

$$\hat{\Theta}_{\text{Improved}} \Psi(v, \phi) = -[B(v)]^{-1} \left\{ C^+(v) \Psi(v+4, \phi) + C^0(v) \Psi(v, \phi) + C^-(v) \Psi(v-4, \phi) \right\} , \quad (4.48)$$

$$C^+(v) := \frac{3\pi K G}{8} |v+2| \left| |v+1| - |v+3| \right| , \quad (4.49)$$

$$C^-(v) := C^+(v-4) , \quad C^0(v) := -C^+(v) - C^-(v) . \quad (4.50)$$

Thus the main changes in the quantization of the Hamiltonian constraint are: (1) replace $\mu_0 \rightarrow \bar{\mu} := \sqrt{\Delta/|p|}$ in the holonomies; (2) *choose* symmetric ordering for the gravitational constraint; and (3) *choose* $j = 1/2$ in both gravitational Hamiltonian and the matter Hamiltonian (in the definition of inverse powers of triad operator). The ‘‘improvement’’ refers to the first point. This model is singularity free at the level of the fundamental constraint equation (even though the leading coefficients of the difference equation do vanish, because the parity symmetry again saves the day); the densities continue to be bounded above – and now with a bound independent of matter parameters; the effective picture continues to be singularity free and with undesirable features removed and the classical Big Bang being replaced by a quantum bounce is established in terms of *physical* quantities.

There is yet another spin on the story of singularity resolution!

4.2.1 Madhavan Quantization [18]:

The improved quantization scheme works primarily through the holonomy corrections, so much so that even if the inverse volume corrections in the matter are turned-off by hand, the singularity resolution continues. Madhavan works within the same kinematical Hilbert space of LQC but treats the Hamiltonian constraint differently, exploiting its specific, simple form for the massless scalar matter. In his quantization of the Hamiltonian constraint, it is the inverse volume corrections that are responsible for singularity resolution (also in terms of physical quantities) and holonomy corrections are by-passed completely.

He observes that the classical Hamiltonian constraint (4.27), is quadratic in c and is of the form of difference of two squares. It can therefore be written as a product,

$$C_{\text{tot}} = -C_+ C_- \quad , \quad C_{\pm} := -\sqrt{\frac{6}{\gamma}} c |p|^{1/4} \pm \sqrt{\kappa} \frac{p_{\phi}}{|p|^{3/4}}$$

The C_{\pm} are linear in c . Since to define physical Hilbert space, a general procedure is to average over the group generated by the constraint, and this involves exponentiation of the constraint, one can directly define these operators which involve factors of the same form as the h_f operators of the improved quantization!

The key differences in Madhavan quantization are: (1) The Hamiltonian constraint is regulated differently from the analogue of LQG and as a consequence, *there are no holonomy corrections* ($\sin^2(c)$). However, the inverse triad corrections can be incorporated in the definition of \hat{C}_{\pm} through the \hat{p}_{ϕ} term. One again uses the volume eigenvalues basis for the inverse triad definition; (2) the physical states are constructed directly by group averaging using the well-defined unitary operators, $e^{i\alpha\hat{C}_{\pm}}$, consequently *there is no difference/differential equation to be solved*; (3) One of the Dirac observables, p_{ϕ} is the same but another one is somewhat different. Nevertheless, *classical solutions* can be derived from their expectation values; (4) The issue of independence from the fiducial cell (discussed in the next subsection) is also addressed differently.

The results are: (i) without inverse triad modifications, the classical (singular) solution is recovered; (ii) with inverse triad modifications, there *is* extension of the solution past the classical singularity with the energy density remaining bounded all through, making the extension non-singular. *There is no bounce, but a regular extension!*

Although Madhavan's procedure of bypassing the holonomy corrections completely, is tied to the particular form of the constraint of the isotropic model (and hence may not extend to other models), it does demonstrate the possibility that there are inequivalent ways of constructing *physical Hilbert space and observables* starting from the *same kinematical structures*. Secondly, singularity resolution *need not* be seen only as a classical/quantum *bounce*, a regular extension is also a distinct possibility.

More details should be seen in [18].

4.2.2 Role of the Fiducial cell in spatially flat models

Recall that in the description of spatially homogeneous and isotropic models one begins with a metric of the form (4.1). The spatial metric is a metric with spatially constant (but possibly time dependent) curvature. This is conveniently taken to be a time dependent scaling of a fixed *co-moving metric* with corresponding *co-moving coordinates*. Although not strictly necessary, let us assign length dimension to the co-moving coordinates and take the scale factor to be dimensionless. For non-flat models the co-moving metric can be normalized to have the Ricci scalar to be ± 1 in appropriate units (Ricci scalar has dimensions of $(\text{length})^{-2}$). Note that this is a *local* condition, and by homogeneity, holds everywhere on the spatial manifold. It is independent of the *size* of the spatial manifold. For flat models, such a normalization of the co-moving metric is not possible. In this case, there is an arbitrariness in the *definition* of the scale factor. Clearly, by focusing only on those quantities which are invariant under constant scaling of the scale factor, eg $\dot{a}/a, \ddot{a}/a$, the energy density etc we

can obviate the need for choosing a co-moving metric/coordinates. The equations of motion - the Friedmann equation and the Raychaudhuri/continuity equation - reflect this feature.

However, spatial flatness, homogeneity and isotropy also implies existence of (global) Cartesian coordinates with a metric $g_{ij}^0 = \delta_{ij}$ with the coordinate differences giving distances in the chosen unit of length. This unit is arbitrary, but also determines the unit of time by putting speed of light to be one. Change in this unit results in an overall scaling of the *space-time metric* but does not affect the scale factor. The scale factor is now unambiguously identified and co-moving coordinates and metric are also fixed.

Construction of a quantum theory of the scale factor degree of freedom (and matter homogeneous degrees of freedom) begins with a *four dimensional action* principle restricted to homogeneous modes of the fields. The action contains a spatial integration which is *divergent* for spatially flat models, thanks to homogeneity. To have a well defined phase space formulation, we need to regulate this divergence. This is done by introducing an *arbitrarily chosen fiducial cell*, specified by finite ranges of the co-moving coordinates (thus having a finite co-moving volume V_0) and restricting the integrations to this cell. Note that this *need and the freedom* in the choice of the fiducial cell arises strictly due to the need for an action formulation for the full theory and the assumption of spatial homogeneity¹³. All subsequent computations will carry a dependence on this cell, either explicitly or implicitly. In the end, this dependence is to be removed by taking a suitable limit $V_0 \rightarrow \infty$ ¹⁴. Precisely at what stage and how should one take the limit?

In the canonical formulation of the full theory, the fiducial volume, V_0 , appears in the symplectic structure. This can however be absorbed away by redefining the canonical coordinates $(\tilde{c}, \tilde{p} \rightarrow c, p)$. This makes the canonical coordinate p to have dimensions of (length)². Note that the physical volume of the cell is $a^3(t) \times V_0$ is now directly given by $|p|^{3/2}$. *Apparently*, there is no reference to the fiducial cell any more in the model. However this is not so. The $|p|^{3/2}$ is the physical volume *of the fiducial cell*. All subsequent computations, whether classical or quantum, done using the (c, p) variables¹⁵ have *no explicit reference* to the cell. For example, the classical solution obtained in terms of phase space trajectory, (eqn. 4.7), does not depend on V_0 .

As discussed above, the subsequent steps in the quantization, do not introduce any further dependence on the fiducial cell. It is no where in sight even in the computation of the phase space trajectory (expectation values of the Dirac observables). These trajectories of course differ from the corresponding classical trajectories. The problem of Big Bang singularity is however phrased in the framework of space-time geometry, specifically, in terms of backward evolution of the *scale factor*. So we need to *transcribe* the phase space trajectories (computed in terms of expectation values of Dirac observables) into evolution of the space-time geometry i.e. the scale factor. At this stage, a scale factor (and an explicit reference to the fiducial cell) is re-introduced via the triad variable as, $a := \xi \sqrt{p}$ where ξ has dimensions of (length)⁻¹ and can be identified with the fiducial volume: $\xi^{-1} = V_0^{1/3}$ (since $p^{3/2}$ is the physical volume *of the fiducial cell*). The phase space evolution then gives $a(t)$. The scale factor evolution

¹³The action formulation (Lagrangian or Hamiltonian) in turn is required for a quantum theory. The classical theory needs only equations of motion which are independent of any cell.

¹⁴The limit $V_0 \rightarrow \infty$ can be viewed as a convenient way to pick-out V_0 -independent terms and/or could also be heuristically motivated by noting that the definition of homogeneity identifies the spatial manifold with the group manifold and this group manifold is \mathbb{R}^3 for the present case.

¹⁵During the process of *loop quantization*, fiducial scales could appear again eg through the holonomies along edges. However as explained in the footnote 3, the V_0 disappear.

so deduced could have some dependence on ξ . After taking the limit $\xi \rightarrow 0$ ($V_0 \rightarrow \infty$), the evolution that survives, is the prediction of the quantum theory, Whether or not this evolution is *singularity free* (i.e. all physical quantities remain bounded through out the evolution) is the central question of interest. Since the phase space curves are inferred from the expectation values, the states in which these are computed are also important to specify. These are expected to be computed in physical states peaked on large volume $p \gg \ell_p^2$ and small energy density (say), corresponding to a classical regime. The singularity free evolution is required to hold for *all* such states.

The classical evolution given in eqn (4.7) provides an example of this transcription. We see that ξ^{-2} cancels out from both p and p_* and the classical evolution of the scale factor is *independent* of the fiducial cell as it should be. The LQC computed solution for p , always shows a bounce, is not very explicitly expressed and also contains an implicit dependence on the fiducial cell. It matches pretty closely with the classical solution in the large p regime and therefore could be expected to be V_0 independent in these regimes. This removes the cell dependence in the initial condition and the question boils down to whether the bounce feature and value of p at the bounce, is independent of V_0 .

The APS investigations[10, 17] found that, in the μ_0 -scheme, a bounce can occur even for low values of energy density something which is not exhibited by the observed isotropic universe. Furthermore, the energy density at the bounce - which is a physical observable - has a V_0 -dependence. So the quantization scheme has some problems. What exactly does this mean?

Note that this does not necessarily mean that there is any mathematical inconsistency in the process of quantization. However, the constructed quantum theory should agree with GR for low energy densities (i.e. have acceptable infra-red behaviour) and hopefully also *imply a non-singular evolution*. It is possible that it may fail this expectation. APS analysis concludes that the μ_0 -scheme with symmetric ordering fails this test.

In retrospect, this failure could have been inferred in the following way. The earlier methods of analysis were based on WKB approximation and effective Hamiltonians[12] derived from it. This allowed us to encode quantum modifications in terms of effective density and effective pressure, defined by computing the left hand sides of the Friedmann and the Raychaudhuri equations using the effective Hamiltonian. In these papers, the scale factor was introduced by setting $p := a^2/4$ (dimensionful) and therefore still refers (implicitly) to fiducial cell. To make the fiducial cell explicit, replace this scale factor as $a \rightarrow a\xi^{-1}$. The expressions for the energy density (say) can be transcribed in terms of the (dimensionless) scale factor and ξ . As explained above, prediction of the quantum theory for the scale factor evolution is obtained by taking the limit $V_0 \rightarrow \infty$ ($\xi \rightarrow 0$). Note that this is now done at the level of equations as opposed to at the level of individual curves which need initial conditions to be chosen (which we have argued to be independent of V_0).

Recall the effective density given in eqn.[4.26],

$$\begin{aligned} \rho_{\text{eff}} &= \left(\frac{H_{\text{matter}}}{p^{3/2}} \right) \left[1 - \frac{2\kappa\mu_0^2\gamma^2}{3} p \left(\frac{H_{\text{matter}}}{p^{3/2}} \right) \right] \quad , \quad \text{where} \\ H_{\text{matter}} &= \frac{1}{2} p_\phi^2 \left\{ (2jp_0)^{-3/2} (F_\ell(q))^{\frac{3}{2(1-\ell)}} \right\} \quad , \quad q := \frac{p}{2jp_0} \end{aligned} \quad (4.51)$$

The square bracket contains the modification implied by *holonomy corrections*¹⁶. The inverse volume corrections are contained in the matter Hamiltonian (see eqns.(4.12, 4.13)).

Consider first the inverse volume corrections. Observe that with $p \rightarrow a^2 \xi^{-2}/4$, $q \sim a^2 \xi^{-2} \gg 1$ in the limit $\xi \rightarrow 0$. The limiting form of F_ℓ then implies that $p^{-3/2} H_{\text{matter}} \sim p_\phi^2 \xi^6 a^{-6}$. For massless scalar matter, the classical equation of state has $P/\rho = 1$ and hence the classical density behaves as $\sim a^{-6}$. Thus $p_\phi^2 \xi^6$ must be a constant for any particular solution. For the leading term to give the classical evolution, we have to take the limit $\xi \rightarrow 0$ *along with* $p_\phi \rightarrow \infty$ keeping $p_\phi \xi^3$ a *constant* specifying a particular initial condition. This understood, the $p^{-3/2} H_{\text{matter}}$ factors go over to the *cell independent* classical density plus corrections down by $q^{-2} \rightarrow 0$ in the limit. Thus, inverse volume *corrections*, simply vanish when $V_0 \rightarrow \infty$ is imposed.

Now consider the holonomy corrections. By the same logic as above, the holonomy corrections, second term in the square bracket in the effective density expression, goes as $\xi^{-2} \rightarrow \infty!$. This is clearly unacceptable. Thus, in the μ_0 scheme of quantization, the inverse volume modifications do not survive the limit while the holonomy modifications give an inconsistency and neither shed any light on the singularity resolution issue.

True as these features are, they are not immediately conclusive to look for alternative quantizations because the fault may be with the WKB approximation and the corresponding effective Hamiltonians. For instance if one took the effective density from the first paper of [12], the holonomy corrections would also be down by inverse powers of q and would vanish which is okay for the classical limit but the extrapolation to the quantum regime is unreliable since WKB is unreliable at turning points. Perhaps, physical level computations would clarify the issue. This is indeed the case. With the physical level computations, APS results show the unacceptability of the μ_0 -scheme while in Madhavan's approach, with no holonomy corrections, the inverse volume corrections would simply vanish by the argument given above. Both APS and Madhavan have also suggested ways out.

The APS analysis discussed above shows that the $\mu_0 \rightarrow \bar{\mu}(p) = \sqrt{\Delta} \ell_P / \sqrt{p}$ substitution in the holonomies used in replacing the c variable, suffices to obtain a non-singular evolution with good infra-red behaviour. It implies that the deviations from classical evolution (eg close to the bounce) occur when the energy density reaches a universal, maximal value. This substitution also renders the inverse triad correction from the matter sector highly suppressed¹⁷.

Madhavan suggests that along with the APS suggested substitution, one should also introduce a multiplicative parameter λ as $\mu_0 \rightarrow \lambda \bar{\mu}(p)$. Since only corrections that drive the quantum modifications are the inverse volume correction and these go as $(\lambda/v_1)^2 \sim (\lambda \xi^3 \ell_P^3 / a^3)^2$ (see eqn 5.45), ξ independence is achieved by choosing $\lambda \sim (\bar{\xi}/\xi)^3$ where the new dimensional parameter $\bar{\xi}$ is supposed to reflect a scale provided by an underlying LQG state supporting the homogeneity approximation. For details, please see [18].

To summarize: For the spatially flat, isotropic models, let us choose the Cartesian coordinates with the standard Euclidean metric for the spatial slice and choose proper time as the time coordinate so that the space-time metric takes the form (4.1). The scale factor is now specified unambiguously. For constructing a quantum theory, we need to choose a regulator

¹⁶In the first paper of [12], the effective density contained only the leading terms of the holonomy corrections which have been summed up in the second paper.

¹⁷From eqn. 5.45, with $\lambda = 1$, one sees that the corrections go as $v_1^{-2} \sim \ell_P^6 p^{-3} \sim \ell_P^6 (\xi)^6 a^{-6} \rightarrow 0$ as $\xi \rightarrow 0$.

cell with volume V_0 . While the cell dependence can be hidden by choosing scaled variables, it manifests again because quantum computed evolution must be transcribed in terms of the scale factor evolution. This is necessary because the classical Big Bang singularity is understood as a singular evolution of the scale factor so its resolution lies in making the evolution non-singular.

The scale factor evolution can be cast in the form of the Friedmann equation with possible deviations from classical evolution, encoded in the effective density. A prediction of the quantum theory is the surviving correction terms after taking the limit $V_0 \rightarrow \infty$. A quantum theory could be understood to have resolved the Big Bang singularity if the surviving evolution is non-singular. Cell independence of quantum corrections automatically implies that non-trivial limit exists. Not every quantization scheme passes this test.

There are two types of corrections - the holonomy corrections and the inverse triad corrections. These have different properties in the limit. The APS quantization with μ_0 -scheme implies that holonomy corrections dominate and lead to unphysical implications. These are cured by the $\bar{\mu}$ -scheme. The Madhavan quantization scheme, even with the $\bar{\mu}$ substitution in the inverse volume definition, these corrections again vanish unless additional λ parameter is introduced. In either case, extra ingredients (scales) have to be ‘imported’ to get non-trivial results. Both the schemes have ingredients (role played by the area operator in the APS scheme¹⁸ and the specific form of constraint in the Madhavan scheme) which do not have counterparts in the full theory as it is understood at present.

So far the discussion has been within the context of full theory being classically reduced directly to a homogeneous and isotropic model. In the next subsection, we briefly discuss how homogeneity and isotropy can be viewed from within a particular quantized inhomogeneous model.

4.2.3 A View from Inhomogeneity

To keep the flow of the in focus, basic details of the inhomogeneous model are given in the appendix 5.4.

The fundamental change in the way homogeneity is viewed, is that it is a property exhibited by a *state* of an inherently (spatially) inhomogeneous model. For definiteness, a lattice model with a lattice spacing ℓ_0 is taken. This allows for *states* of the model which can be considered as *homogeneous on a certain scale*, eg $\ell_0 N^{1/3}$. This also allows the fields to be restricted to be periodic on this scale. Thus what is fundamental is the lattice spacing ℓ_0 below which it makes no sense to consider inhomogeneity (or inhomogeneities are not probed) and a scale $N^{1/3}\ell_0$ provided by a state of the model. Let us call the former as the *micro-scale* and the latter as the *macro-scale*. The fundamentally isotropic model refers to the macro-scale. The fiducial cell of the isotropic model is determined by these two scales with fiducial volume given by, $V_0 := N\ell_0^3$. Notice that in this view, V_0 (or N) is a property of a quantum state and there is *no reason* to contemplate a limit $V_0 \rightarrow \infty$.

Now all quantum effects due to inverse volume and holonomies, arise at the micro-scale. To see how these translate or correspond to the quantum effects seen in the fundamentally

¹⁸The logic used to motivate the role of area operator, is also extended to other Bianchi models such that when isotropy is imposed, the $\bar{\mu}$ -scheme of isotropic model is recovered back[21].

isotropic model, let us begin by identifying variables.

In the lattice model, isotropic connection is defined by $\tilde{k}(x) = \tilde{c}, \forall x, I$. Identifying this constant value with \tilde{c}_{iso} and comparing the basic link holonomies with the holonomies of the isotropic model implies,

$$c_{\text{iso}} := V_0^{1/3} \tilde{c}_{\text{iso}} = V_0^{1/3} \tilde{k}_I := V_0^{1/3} \ell_0^{-1} c_{\text{lat}} = N^{1/3} c_{\text{lat}} \quad (4.52)$$

The first equality is the definition from the isotropic model, the second one identifies the isotropic connection with the lattice connection \tilde{k} , the third one defines c_{lat} and fourth equality gives the final relation between the ‘ c ’ variables of the isotropic and the lattice models.

The state exhibiting isotropy on the macro-scale, may be characterised by stipulating that the $\tilde{p}_I(\vec{v})$ values are all mutually equal, and equal to \tilde{p}_{lat} , for the vertices comprising the fiducial cell and that this value is identified with the isotropic variable, \tilde{p}_{iso} . Recall that the isotropic operator is obtained by an averaging of the lattice operators. The stipulation says that the average value is realized at each of the lattice vertices. This leads to,

$$p_{\text{iso}} := V_0^{2/3} \tilde{p}_{\text{iso}} = V_0^{2/3} \tilde{p}_{\text{lat}} = V_0^{2/3} p_{\text{lat}} \ell_0^{-2} = p_{\text{lat}} N^{2/3} \quad (4.53)$$

These identification give a relation between isotropic variables and a state of lattice model with a scale parameter N . A dynamically evolving isotropic universe may be thought of as a family of lattice states with the scale N being a function of the volume eg larger number of elementary cells get ‘homogenised/isotropised’. As an example, if $N \propto p_{\text{iso}}^{3/2}$, then p_{lat} will be a constant! The expressions seen in the context of isotropic models with fiducial cell of size V_0 are now to be applied to the elementary cell of size ℓ_0^3 .

In view of these identifications, let us consider the two specific corrections seen in the isotropic model, namely the the inverse volume corrections and the holonomy corrections. In the lattice model, these corrections arise in the same manner as in the isotropic model, but from the micro-cell. The inverse volume corrections are in powers of $p_*/p = p_*/p_{\text{lat}} = (p_*/p_{\text{iso}})N^{2/3}$. For $N \propto p_{\text{iso}}^{3/2}$, these are independent of p_{iso} . (ii) With the holonomy corrections included, the effective density (4.51), is of the form $\rho(1 - \rho/\rho_{\text{crit}})$ with $\rho_{\text{crit}}^{-1} \sim \kappa\gamma^2 p_{\text{lat}} = \kappa\gamma^2 p_{\text{iso}} N^{-2/3}$. Again for $N \propto p_{\text{iso}}^{3/2}$, ρ_{crit} is independent of p_{iso} . For a different dependence of N on p_{iso} , the corrections will have non-trivial dependence on p_{iso} and therefore on V_0 , but V_0 is no longer a purely mathematical artifact but is dictated by the underlying inhomogeneous state.

In effect, a perspective from an underlying inhomogeneous model suggests that the fiducial cell of a homogeneous model is selected by a state of the inhomogeneous model and a dependence on the $V_0 := \ell_0^3 N$ is not necessarily unphysical. For a more detailed discussion of ramifications of these ideas, please see [16].

Chapter 5

Appendix

5.1 Symmetric connections

We assume that we have a manifold M on which are defined connection $A_\mu^a(z)$ with a taking values in the Lie algebra \underline{G} of a *gauge group* G . Assume further that there is an action of a *symmetry group* S on M under which we want to have appropriate notion of invariance. The infinitesimal action of the symmetry group is generated by a set of vector fields $\xi_m^\mu \partial_\mu$ which represent the Lie algebra of S : $[\xi_m, \xi_n] = f_{mn}^p X_p$. The Lie algebra of G is generated by matrices T_a satisfying: $[T_b, T_c] = C_{bc}^a T_a$.

When we have an ordinary tensor field, T , on a manifold, it is defined to be invariant under (or symmetric w.r.t.) the action of an infinitesimal diffeomorphism generated by a vector field ξ if its Lie derivative with respect to ξ vanishes: $L_\xi T = 0$. When the tensor fields also transform under the action of a gauge group, then the invariance condition allows the Lie derivative to be an infinitesimal gauge transform of the tensor field: $L_\xi T = \delta_{W(\xi)} T$, where $W(\xi)$ is valued in the Lie algebra \underline{G} . Notice that this associates a gauge transformation with a diffeomorphism.

This association has to satisfy two conditions: (a) If we took a gauge transform of the tensor field and then applied the diffeomorphism, the defining condition must be gauge covariant: $L_\xi(T^g) = \delta_{W^g(\xi)} T$, where $W^g(\xi) = g^{-1} W(\xi) g + g^{-1} L_\xi(g)$, and (b) The Lie derivatives represent the Lie algebra of the symmetry group: $[L_{\xi_m}, L_{\xi_n}] T = L_{[\xi_m, \xi_n]} T = f_{mn}^p L_{\xi_p} T$ and the W_m must obey the consequent conditions. The task is to find those tensor fields which satisfy the invariance conditions subject to the allowed gauge transformations.

This is aided by another consequence of the symmetry action. The action of the the symmetry group S on M implies that M can be expressed as a collection of *orbits* of S . We will assume the simpler case where *all* orbits are mutually diffeomorphic and are given by S/F where F is the stability subgroup of the S -action. Thus we obtain $M \sim B + S/F$. Here S/F is an orbit which is necessarily a coset space while B is a manifold whose points label the orbits. Note that a non-trivial subgroup F of S means that a subset of vector fields ξ_m vanish at some point. Corresponding to this structure of M , its tangent and cotangent spaces are also decomposed.

The solutions of the invariance conditions are constructed by using the available structure on the group manifold S and projecting these onto S/F . Here are some details for the gauge

connection¹ [22].

Let $A := A_\mu^a T_a dx^\mu$ denote the \underline{G} valued connection 1-form (the gauge potential). Under a gauge transformation it transforms as: $A^g := g^{-1} A g + g^{-1} dg$ and infinitesimally, $g = 1 + \epsilon W$, $\delta_{\epsilon W} A = \epsilon D(W) := \epsilon(dW + [A, W])$, $W := W^a T_a$. Under an infinitesimal diffeomorphism, $x'^\mu := x^\mu + \epsilon \xi^\mu$, it transforms as $\delta_{\epsilon \xi} A := -\epsilon L_\xi A = -\epsilon(\partial_\mu \xi^\nu A_\nu + \xi^\nu \partial_\nu A_\mu) dx^\mu = -\{i_\xi dA + d(i_\xi A)\}$.

The invariance conditions, when there are many symmetries, are:

$$L_{\xi_m} A = D(A) W_m := dW_m + [A, W_m] \Leftrightarrow \partial_\mu \xi^\nu A_\nu + \xi^\nu \partial_\nu A_\mu = \partial_\mu W_m + [A_\mu, W_m] . \quad (5.1)$$

Here, W_m are some \underline{G} valued scalars on the manifold M associated with ξ_m . We induce a gauge transformation on the W_m by demanding that the above condition be *gauge covariant*:

$$L_{\xi_m} A^g := D(A^g) W_m^g \Leftrightarrow W_m^g := g^{-1} W_m g + g^{-1} L_{\xi_m} g , \quad L_{\xi_m} g := \xi_m^\mu \partial_\mu g \quad (5.2)$$

The Lie algebra of the vector fields, ξ_m , implies that the W_m 's must satisfy:

$$\begin{aligned} [L_{\xi_m}, L_{\xi_n}] A &= L_{[\xi_m, \xi_n]} A = f_{mn}^p L_{\xi_p} A && \Rightarrow \\ D(W_{mn}) &= f_{mn}^p D(W_p) , \quad W_{mn} := L_{\xi_m} W_n - L_{\xi_n} W_m + [W_m, W_n] , && \text{or} \\ 0 &= D(W_{mn} - f_{mn}^p W_p) && (5.3) \end{aligned}$$

where $[W_m, W_n]$ is the bracket in the Lie algebra, \underline{G} .

Exercise: For the field strength $F_{\mu\nu}^a T_a$, verify that $L_{\xi_m} F = [F, W_m]$.

Exercise: Let E be a vector field valued in \underline{G} which transforms as $E^g = g^{-1} E g$. The condition for symmetric E would be $L_{\xi_m} E = [E, W_m]$. Show that the W_m transforms as before and the symmetry Lie algebra implies $[E, W_{mn} - f_{mn}^p W_p] = 0$.

Suppose that $\chi_{mn} := W_{mn} - f_{mn}^p W_p \neq 0$. Then the above equations imply conditions on symmetric field strength (and indeed on all symmetric quantities). For example, $D\chi_{mn} = 0$ implies that $[F, \chi_{mn}] = 0^2$. This would mean that the field strengths must commute with the χ_{mn} 's. We will assume that there does not exist any χ valued in \underline{G} such that $D\chi = 0$. This implies that $\chi_{mn} = 0$ i.e.

$$L_{\xi_m} W_n - L_{\xi_n} W_m + [W_m, W_n] - f_{mn}^p W_p = 0 . \quad (5.4)$$

Note that this is a condition involving only the W_n 's and the symmetry generators ξ_m 's. Also observe that for vector fields corresponding to the stability subgroup F , the (5.4) reduces to $[W_m, W_n] = f_{mn}^p W_p$ at the points where these vector fields vanish.

The task is to characterise the symmetric connections satisfying eqn. (5.1) with W_n satisfying eqn. (5.4) modulo gauge transformations (5.2) on a manifold $M \sim B \times S/F$. The strategy is to show that the gauge freedom allows W_n to be taken in appropriate form and then determine the form of symmetric connections in the same gauge.

¹In the context of Kaluza-Klein approach to unification, the analysis of invariant quantities was carried out to construct suitable ansatz. There, the space-time is taken to be of the product form $M_4 \times B$ with B a compact manifold. The isometry groups of the compact manifold played the role of symmetries and the forms of the fields on the space-times were obtained.

²Note that $D\chi = 0$ follows only for the symmetric connections. If it were to hold for all connections, then $[F, \chi] = 0$ would hold for all field strengths and this would correspond to a reduction of the gauge group to the little group of χ_{mn} . This is analogous to the non-trivial Higgs vacua situation.

Consider first the case where $F = \{e\}$ so that $S/F = S$ itself. Introduce local coordinates (x^i, y^α) on $B \times S$. Without loss of generality, we can take the symmetry generators to be functions of y and with zero components along B . Noting that the vector fields ξ_m on S are independent, it follows that the matrices $\xi_m^\alpha(y)$ are invertible and therefore we can define new \underline{G} valued 1-forms as: $W_m(x, y) := \xi_m^\alpha W_\alpha(x, y)$. It is easy to see that (i) W_α transform exactly as a G -connection and (ii) the condition (5.4) is just the statement that this connection is flat. Therefore, *locally* it is always possible to choose $W_\alpha(x, y) = 0$ and hence $W_m(x, y) = 0$. Having chosen W_m 's to be zero, the gauge transformation freedom is restricted to $L_{\xi_m}(g) = \xi_m^\alpha \partial_\alpha g = 0$ i.e. the gauge functions must depend only on the x coordinates.

In this gauge, the invariance conditions can be written separately for $\mu = i$ and for $\mu = \alpha$ as:

$$\xi_m^\alpha \partial_\alpha A_i = 0 \quad \text{and} \quad (L_{\xi_m} A)_\alpha = 0$$

The first implies that A_i depends only on x and so do the gauge transformations. Hence A_i is a G -connection on B . The solution for A_α is obtained as follows.

On a group manifold, there are left and right actions of the group onto itself which commute. Consequently, these generate left(right) invariant vector fields and 1-forms (the Maurer-Cartan forms). Apply these to the group manifold S . Assume that ξ_m generate *left* action on the group manifold and use the *left* invariant 1-forms eg the unique, \underline{S} -valued Maurer-Cartan form Θ_{MC} ³. It is immediate that $L_{\xi_m} \Theta_{MC} = 0$. To obtain a G -connection, we need a map $\Lambda : \underline{S} \rightarrow \underline{G}$. Given such a map, we can define $A := \Lambda(\Theta_{MC}) \leftrightarrow A_\alpha^a := \Phi_m^a(\Theta_{MC})_\alpha^m$. Now $L_{\xi_m} A = 0 = L_{\xi_m}(\Phi)\Theta_{MC} + 0$ implies that the ‘‘Higgs’’ fields, Φ_m are constants on S i.e. are functions only of x^i .

Thus, for the case where the S -action is free (F is trivial), the symmetric connections can be written as $A = \mathcal{A}_i(x)dx^i + \Phi_m(x)\omega_\alpha^m(y)dy^\alpha$ where \mathcal{A} is an arbitrary G -connection on B and $\Phi_m(x)$ are ‘‘Higgs’’ scalars valued in \underline{G} .

When the S -action is not free, the vector fields ξ_m^α are tangent to S/F and the above steps do not go through immediately. Nevertheless we can still find invariant, \underline{S} -valued 1-forms on S/F and a suitable map Λ to construct invariant connections. To see this, note that there is the natural projection map $\pi : S \rightarrow S/F$. Choose an *embedding* $i : S/F \rightarrow S$. As discussed above, on S we have vector fields $\bar{\xi}_m$ generating left action and the corresponding Maurer-Cartan form Θ_{MC} . Using π_* we push-forward the vector field on to S/F and using i^* we pull-back Θ_{MC} on to S/F . The projected vector fields match with the ξ_m (by definition of the symmetry action). Thus we get,

$$\xi_n := \pi_*(\bar{\xi}_n) \quad , \quad \omega := i^*(\Theta_{MC}) \quad ; \quad L_{\bar{\xi}_n} \Theta_{MC} = 0 \quad \Rightarrow \quad L_{\xi_n} \omega = 0 .$$

As before, ω is valued in \underline{S} since Θ_{MC} is. Introduce Φ_n^a as before and define $A_\alpha^a := \Phi_n^a \omega_\alpha^n$. Using these definitions let us rewrite the defining equations as:

$$\text{Invariance condition} \quad : \quad (\xi_n^\alpha \omega_\alpha^k) (L_{\xi_m} \Phi_k - [\Phi_k, W_m]) = L_{\xi_n} W_m ; \quad (5.5)$$

$$\text{Lie Algebra condition} \quad : \quad L_{\xi_m} W_n - L_{\xi_n} W_m - [W_m, W_n] = f_{mn}^p W_p ; \quad (5.6)$$

$$\text{Gauge transformations} \quad : \quad W_m^g = g^{-1} W_m g + g^{-1} L_{\xi_m} g ; \quad (5.7)$$

$$: \quad (\xi_n^\alpha \omega_\alpha^k) (\Phi_k^g - g^{-1} \Phi_k g) = g^{-1} L_{\xi_n} g \quad (5.8)$$

³For classical matrix groups, these are given by $g^{-1}dg$ and $dg g^{-1}$ and are left and right invariant respectively.

In writing the first equation we have used $L_{\xi_m} \omega^n = 0$ and also multiplied by ξ_n^α .

The last equation implies that Φ_n 's transform as the adjoint representation of G iff the gauge transformations are constant over S/F . We can take Φ_n to transform by the adjoint representation of G , thereby restricting the gauge transformation to be constant over S/F . In such a case, W_n 's also transform the same way. For trivial F , we can transform away W_n to zero and recover the previous case. For non-trivial F , this is not the case.

For non-trivial F , there exist a point, y_0 say, in S/F at which the vector fields $\xi_{\underline{m}}, \underline{m} = 1, \dots, \dim(F)$ vanish. Then $L_{\xi_{\underline{m}}}$ terms drop out. Consider the equation (5.6) for $\underline{m}, \underline{n}$. Then, at y_0 , we must have $[W_{\underline{m}}, W_{\underline{n}}] = f_{\underline{mn}}^p W_{\underline{p}}$. Since F is a subgroup, the sum on the right hand side is restricted to \underline{p} . If there is a non-trivial homomorphism $\lambda : F \rightarrow G$, it will induce a corresponding homomorphism $\Lambda : \underline{F} \rightarrow \underline{G}$ on the Lie algebras and we can choose the $W_{\underline{m}}(y^0)$ to represent it.

Next, at y_0 , consider the (5.5,5.6) for \underline{m} . Eliminating $L_{\xi_n} W_{\underline{m}}$, and noting that Φ_k alone depends on x , we must have (a) $[W_{\underline{m}}, W_n] = f_{\underline{mn}}^p W_{\underline{p}}$ and (b) $[\Phi_n, W_{\underline{m}}] = 0$. Note that this implies that the residual gauge group is reduced to those elements of G which commute with $W_{\underline{m}}$ i.e. to the *centralizer of $\lambda(F) \subset G$* . The gauge transformations are already restricted to be functions of x alone.

Considering the Jacobi identity for $\Phi_{\underline{k}}, \Phi_l, W_{\underline{m}}$ it follows that $[\Phi_{\underline{k}}, \Phi_l] = d_{\underline{kn}}^m \Phi_m$ must hold for some d 's. This has the same form as the condition (a) on the W 's. Hence $d_{\underline{kl}}^m = f_{\underline{kl}}^m$ is obviously a solution.

In fact, it is a result that S -invariant connections, when they exist, are in on-to-one correspondence with homomorphisms of the groups $\lambda : S \rightarrow G$ and can be expressed as $A(x, y) = \mathcal{A}_i dx^i + \Phi(x)_n i^* (\Theta_{MC})^n(y)$ where \mathcal{A} is a connection on B with the gauge group *reduced to the centralizer of $\lambda(F)$ in G* (i.e. group of all elements of G which commute with the image of F in G under the homomorphism λ). Furthermore the Higgs fields have to satisfy the constraints: $[\Phi_{\underline{m}}, \Phi_n] = f_{\underline{mn}}^p \Phi_p$ ⁴.

What about other invariant fields, such as vector fields in the adjoint of the gauge group (eg the triad fields)? Now the invariance condition (5.5) will change and also the corresponding gauge transformations of the field. For $E_a^\mu \partial_\mu$, we will have $L_{\xi_m} E = [E, W_m], E^g = g^{-1} E g$. Now use the projections X_m of the *left invariant vector fields* \bar{X}_m on S (these generate the right action and are dual to the Θ_{MC}) and write: $E_a^\alpha := \Psi_n^\alpha X_n^\alpha, L_{\xi_m} X_n = 0$. The invariance condition then becomes $(\omega_\alpha^k X_n^\alpha)(L_{\xi_m} \Psi^n - [\Psi^n, W_m]) = 0$ and $(\omega_\alpha^k X_n^\alpha)((\Psi^n)^g - g^{-1} \Psi^n g) = 0$. The gauge transformations imply Ψ^n transforms by the adjoint representation and for $m = \underline{m}$, the invariance condition implies: $[\Psi_n, W_{\underline{m}}] = 0$. Exactly as before, the Ψ^n must satisfy constraints analogous to the Φ_n 's. Similar logic will hold for other tensor fields.

As a very simple illustration, consider the case of static magnetic field in three dimensions invariant under translations along the z-axis. We want to obtain the form of the vector potential A_i . In this case, the gauge group $G = U(1)$ and the symmetry group $S = \mathbb{R}$ which acts on \mathbb{R}^3 by translations. This action is free and therefore $F = \{e\}$. We have $\mathbb{R}^3 \sim \mathbb{R}^2 \times \mathbb{R}$. The Maurer-Cartan form on \mathbb{R} is just dz . The map from $\underline{\mathbb{R}} \rightarrow \underline{U(1)}$ is given by a single 'Higgs' scalar, $\Phi(x, y)$. The symmetric connection is then given by $A_i(x, y, z) dx^i =$

⁴The classification of connections invariant under some group of automorphisms of appropriate bundles is given by *generalised Wang theorem*. There are many mathematical fine prints in the above discussion which should be seen in the references in [23].

$\mathcal{A}_x(x, y)dx + \mathcal{A}_y(x, y)dy + \phi(x, y)dz$. This just says that all the three components of the vector potential depend *only* on (x, y) . Note that this is a statement in the gauge where “ W ” has been set to zero. This implies that the magnetic field is also independent of z . Note that since $A_z := \phi(x, y) \neq 0$, the magnetic field could be along any fixed direction.

Exercise: Work out spherically symmetric Yang-Mills fields in three dimensions. Now $G = SU(2)$, $S = SO(3)$, $F = U(1)$, $\mathbb{R}^3 \sim \mathbb{R}^+ \times S^2$.

Further examples may be seen in [23].

5.2 Schrodinger and Polymer Quantization

We illustrate inequivalent quantization as well as the GNS procedure in a simple example.

5.2.1 The Weyl-Heisenberg C*-Algebra

Consider the usual Schrodinger quantization of a single degree of freedom. We have the usual Hilbert space $L^2(\mathbb{R}, dx)$, on which are defined the self-adjoint operators x, p , satisfying the canonical commutation relations: $[x, p] = i\hbar$.

Define the corresponding unitary operators:

$$\begin{aligned} U(\alpha) &:= e^{i\alpha x} \quad , \quad V(\beta) := e^{i\hbar^{-1}\beta p} \quad , \quad \alpha, \beta \in \mathbb{R} \\ U^\dagger(\alpha) &= e^{-i\alpha x} = U(-\alpha) = U(\alpha)^{-1} \quad , \quad V^\dagger(\beta) = e^{-i\hbar^{-1}\beta p} = V(-\beta) = V(\beta)^{-1} \end{aligned} \quad (5.9)$$

Using the BCH formula,

$$e^A \cdot e^B = e^{A+B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] - \frac{1}{12}[B, [A, B]] + \dots}$$

it follows,

$$U(\alpha)U(\alpha') = U(\alpha + \alpha') \quad , \quad V(\beta)V(\beta') = V(\beta + \beta') \quad , \quad U(\alpha)V(\beta) = e^{-i\alpha\beta}V(\beta)U(\alpha) \quad (5.10)$$

Define, for $z := (\alpha + i\beta)/\sqrt{2} \in \mathbb{C}$, the unitary operator,

$$\begin{aligned} W(z) &:= e^{i\frac{\alpha\beta}{2}}U(\alpha)V(\beta) &= e^{i(\alpha x + \hbar^{-1}\beta p)} \\ &= \exp \left[i \left\{ \frac{z + \bar{z}}{\sqrt{2}} x - i \frac{z - \bar{z}}{\sqrt{2}} \frac{p}{\hbar} \right\} \right] &= \exp \left[i \left\{ z \frac{x - ip/\hbar}{\sqrt{2}} + \bar{z} \frac{x + ip/\hbar}{\sqrt{2}} \right\} \right] \\ &= e^{i(z a^\dagger + \bar{z} a)} &= e^{-\frac{|z|^2}{2}} e^{i z a^\dagger} e^{i \bar{z} a} \quad \text{where,} \end{aligned} \quad (5.11)$$

$$a := \frac{1}{\sqrt{2}} \left(x + i \frac{p}{\hbar} \right) \quad \Rightarrow \quad [a, a^\dagger] = 1 \quad . \quad (5.12)$$

It follows,

$$\begin{aligned} W(z_1)W(z_2) &= e^{-\frac{i}{2}(\alpha_1\beta_2 - \alpha_2\beta_1)}W(z_1 + z_2) \\ &= e^{\frac{1}{2}(z_1\bar{z}_2 - z_2\bar{z}_1)}W(z_1 + z_2) \\ &= e^{\frac{1}{2}\text{Im}(z_1\bar{z}_2)}W(z_1 + z_2) \quad \text{and,} \end{aligned} \quad (5.13)$$

$$W(z)^\dagger = W(-z) = W(z)^{-1} \quad . \quad (5.14)$$

Taking finite linear combinations of products of the unitary operators $W(z)$, we get an algebra called the *Weyl-Heisenberg algebra*, \mathcal{W} . This is $*$ -algebra due to the Hermitian dagger defined for the operators. The unitary operators $W(z)$ are bounded and so are polynomials in them. With respect to the operator norm (which satisfies $\|A^\dagger\| = \|A\|$, $\|A^\dagger A\| = \|A\|^2$), The Weyl-Heisenberg algebra is a C^* -algebra. Notice that the \mathcal{W} C^* -algebra is *non-commutative* and has two *commutative* sub-algebras, namely those generated by the elements, $W(\frac{\alpha+i0}{\sqrt{2}})$ and $W(\frac{0+i\beta}{\sqrt{2}})$ respectively.

Thus at this stage we have constructed a C^* -algebra of bounded operators on the specific Hilbert space. We will now define a *positive linear functional* on the C^* algebra, \mathcal{W} , construct a unitary representation of the algebra and show its equivalence to that provided by the Schrodinger quantization. The same procedure will then be used to construct another representation, the *Polymer Representation*, of the same algebra.

5.2.2 Re-construction of the Schrodinger Representation

In the Hilbert space, consider the wavefunction, $\langle x|0\rangle := \psi_0(x) := \pi^{-1/4}e^{-x^2/2}$ so that $\langle 0|0\rangle := \int dx |\psi_0(x)|^2 = 1$. Following results hold:

$$a|0\rangle = \frac{1}{\sqrt{2}} \left(x - \frac{d}{dx} \right) \psi_0(x) = 0 \quad (5.15)$$

$$\begin{aligned} [W(z)\psi_0](x) &= e^{\frac{i}{2}\alpha\beta} [U(\alpha)V(\beta)\psi_0](x) = e^{\frac{i}{2}\alpha\beta} e^{i\alpha} [V(\beta)\psi_0](x) \\ &= e^{\frac{i}{2}\alpha\beta} e^{i\alpha x} \psi_0(x + \beta) \end{aligned} \quad (5.16)$$

$$\langle x|W(z)|0\rangle = e^{-\frac{|z|^2}{2}} \langle x|e^{iza^\dagger}|0\rangle := \langle x|z\rangle \quad (5.17)$$

$$\begin{aligned} \therefore \int dx \psi_0^*(x) [W(z)\psi_0](x) &= \pi^{-1/2} \int dx e^{-\frac{x^2}{2}} e^{i\alpha x - \frac{(x+\beta)^2}{2}} \\ &= e^{-\frac{|z|^2}{2}} := \langle 0|W(z)|0\rangle = \langle 0|z\rangle \end{aligned} \quad (5.18)$$

Define a linear functional Ω_{Sch} , on the Weyl-Heisenberg algebra

$$\Omega_{\text{Sch}} \left(\sum_i c_i W(z_i) \right) := \sum_i c_i \Omega_{\text{Sch}}(W(z_i)) := \sum_i c_i \langle 0|W(z_i)|0\rangle := \sum_i c_i e^{-|z_i|^2/2} .$$

The first definition ensures linearity and the third one completes the definition. The second definition (notational) makes it obvious that Ω_{Sch} is a positive linear functional since $\Omega_{\text{Sch}}(A^*A) = \langle 0|A^\dagger A|0\rangle = \|A|0\rangle\|^2 \geq 0, \forall A := c_i W(z_i) \in$ the C^* -algebra. The equality holds only if $A|0\rangle = c_i |z_i\rangle = 0$. Since $|z_i\rangle$ states are linearly independent, there are no non-trivial states in the Hilbert space which satisfy $A|0\rangle = 0$. The positive linear functional then defines an *inner product* on the algebra by,

$$\langle W(z), W(z') \rangle := \Omega_{\text{Sch}}(W(z)^\dagger W(z')) = \langle 0|W(-z)W(z')|0\rangle = e^{-\frac{\text{Im}(zz')}{2}} \langle 0|z' - z\rangle .$$

and extended by linearity to the algebra. This turns the algebra into a Hilbert space (distinct from the original Hilbert space).

Next, define operators, $\hat{W}(z)$ acting on the algebra, by,

$$\hat{W}(z)[W(z')] := W(z)W(z') = e^{\frac{\text{Im}(z\bar{z}')}{2}}W(z+z')$$

and extended to the algebra by linearity. Similarly, one defines an operator for each element of the algebra, in an obvious manner.

Exercise: Show that $(\widehat{W(z)})^\dagger = \hat{W}(-z)$.

This implies that $\hat{W}(z)$ are unitary operators.

That $W(z) \rightarrow \hat{W}(z)$ provides a homomorphism of the \mathcal{W} algebra is obvious from the action of the operators. Thus the algebra with the inner product defined, carries a representation of itself in which the $W(z)$ are represented unitarily.

Consider general matrix elements of the operators $\hat{W}(z)$:

$$\begin{aligned} \left\langle W(z_1), \hat{W}(z)[W(z_2)] \right\rangle &= \langle 0|W(-z_1)W(z)W(z_2)|0\rangle \\ &= e^{\frac{1}{2}(z\bar{z}_2 - z_1\bar{z} - z_1\bar{z}_2)} \langle 0|W(z+z_2-z_1)|0\rangle \\ &= e^{\frac{(z\bar{z}_2 - z_1\bar{z} - z_1\bar{z}_2)}{2}} e^{-\frac{|z+z_2-z_1|^2}{2}} \end{aligned} \quad (5.19)$$

Observe that for $z = \alpha$ or $z = i\beta$, the above matrix elements are continuous in α, β respectively. General matrix elements are obtained from finite combinations of these and hence *the* $\hat{W}(\alpha)$ and $\hat{W}(i\beta)$ are both weakly continuous families of unitary operators. Actually, these are also *strongly* continuous families i.e. w.r.t. vector space norm. The strong continuity can be checked by evaluating the norm $\|(\hat{W}(z) - \hat{W}(0))[W(z')]\|$ and checking the limits for $z = \alpha/\sqrt{2}$ and $z = i\beta/\sqrt{2}$.

This allows us to define two self-adjoint operators (on the algebra) as,

$$\hat{X} := \lim_{\alpha \rightarrow 0} \frac{\hat{W}(\alpha/\sqrt{2}) - \mathbb{I}}{i\alpha}, \quad \hat{P} := \hbar \lim_{\beta \rightarrow 0} \frac{\hat{W}(i\beta/\sqrt{2}) - \mathbb{I}}{i\beta} \quad (5.20)$$

$$\implies [\hat{X}, \hat{P}] = i\hbar\mathbb{I} \quad (5.21)$$

The commutator can be evaluated directly using the definitions for $\alpha, \beta \neq 0$ and using the existence of the limits guaranteed by strong continuity.

5.2.3 Another positive linear functional and the Polymer representation:

Now view the Weyl-Heisenberg algebra defined above as an abstract structure i.e. an algebra generated by elements $W(z), z \in \mathbb{C}$, obeying the relations (5.13,5.14) with a norm defined by $\|W(z)\| = 1 \forall z \in \mathbb{C}$ and extended by linearity. Define a linear functional by,

$$\Omega_{\text{Poly}}(W(z)) := \begin{cases} 1 & \text{if } \text{Im}(z) = 0 \\ 0 & \text{otherwise} \end{cases} \quad (5.22)$$

This is positive because

$$\begin{aligned} \Omega_{\text{Poly}} \left(\sum_i \{C_i W(z_i)\}^\dagger \sum_j \{C_j W(z_j)\} \right) &= \sum_{ij} C_i^* C_j e^{-\frac{1}{2} \text{Im}(z_i \bar{z}_j)} \Omega_{\text{Poly}}(W(z_j - z_i)) \\ &= \sum_i |C_i|^2 + \sum_{i \neq j} C_i^* C_j e^{\frac{i}{2} \beta_i (\alpha_j - \alpha_i)} \delta_{\beta_i, \beta_j} \end{aligned} \quad (5.23)$$

In the sum, only those pairs (i, j) which have the same β , contribute. Group together all the terms whose β_i are equal (eg $\{z_1, z_2, \dots, z_m\}, \{z_{m+1}, \dots, z_{m+n}\} \dots$), and consider one such group at a time. In each such group, the phases in the second term can be absorbed in the C_i 's (since the β is common) and then combining with the first term gives $|\sum_i \{C_i e^{i\beta\alpha_i/2}\}|^2$ which is non-negative. This completes the proof. Note that positive linear functional must evaluate to 1 on the identity element of the algebra (namely, $\mathbb{I} := W(0)$) and therefore we *cannot* interchange $\beta \leftrightarrow \alpha$ in the defining condition in (5.22).

The Ω_{Poly} defines a *degenerate* inner product on the algebra,

$$\langle W(z'), W(z) \rangle := \Omega_{\text{Poly}}(W(z')^\dagger W(z)) = e^{-\frac{\text{Im}(z' \bar{z})}{2}} \Omega_{\text{Poly}}(W(z - z'))$$

and extended by linearity. The elements whose norm w.r.t. this degenerate inner product is zero, forms a closed subspace \mathcal{N} , of the algebra and consists of elements of the form $\chi := \sum_i C_i W(\frac{\alpha_i + i\beta}{\sqrt{2}})$, $\beta \in \mathbb{R}$ such that $\sum_i C_i e^{-i\beta\alpha_i/2} = 0$. Elements of \mathcal{N} also satisfy the property: $\Omega_{\text{Poly}}(A\chi) = 0 \forall A \in \mathcal{W}$, which is useful in the exercise below. The quotient space, \mathcal{W}/\mathcal{N} , is an inner product space and its Cauchy completion defines a Hilbert space of the *Polymer Representation*.

Exercise: Let A denote a general element of the algebra and χ an element of \mathcal{N} . Define $[A] := \{B \in \mathcal{W}/B = A + \chi\}$. Define $\langle [A], [B] \rangle := \langle A, B \rangle$ and $\hat{W}(z)\{[A]\} := [\hat{W}\{A\}]$. Show that these definition are well defined and conclude that \mathcal{W}/\mathcal{N} provides a *unitary* representation of the quotient algebra. From now on, we refer to the quotient representation without being explicit about it.

Observe that Ω_{Poly} is continuous in α and *discontinuous* in β . This directly implies that $\hat{W}(i\beta/\sqrt{2})$ *cannot be weakly continuous* and therefore we cannot define the analogue of \hat{P} . This follows by noting that $\langle W(z'), \hat{W}(i\beta/\sqrt{2})\{W(z')\} \rangle \sim \Omega_{\text{Poly}}(W(i\beta/\sqrt{2} + z' - z'))$. The weak continuity (actually also *strong continuity*) in α however allows the definition of \hat{X} self-adjoint operator. It remains to make the representation explicit.

In both the cases above, with the Schrodinger and the polymer functionals, we constructed a representation of the \mathcal{W} in which the $W(z)$ are represented by unitary operators. This is the Gelfand-Naimark-Segal (GNS) construction. In the Schrodinger case, we obtained the \hat{X}, \hat{P} operators satisfying the canonical commutation relations. In the Polymer case we obtained only \hat{X} . In both cases we get the following relations, directly by applying the definitions:

$$\hat{W}^\dagger \left(i\beta/\sqrt{2} \right) \hat{X} \hat{W} \left(i\beta/\sqrt{2} \right) = \hat{X} - \beta \mathbb{I} \Rightarrow \quad (5.24)$$

$$\hat{X} \hat{W} \left(i\beta/\sqrt{2} \right) - \hat{W} \left(i\beta/\sqrt{2} \right) \hat{X} = -\beta \hat{W} \left(i\beta/\sqrt{2} \right) \quad (5.25)$$

From these relations follow an important result. Note that \hat{X} is a self adjoint operator and therefore its spectrum is real. What can one say about its eigenvectors? The above relation

implies that if $|x\rangle$ is an eigenvector of \hat{X} with eigenvalues x , then $\hat{W}(i\beta/\sqrt{2})|x\rangle$ is also an eigenvector with eigenvalues $(x + \beta)$. Hence, either every real number is an eigenvalue or none is.

Suppose every x is an eigenvalue. Then we have the orthogonality relation $\langle x|x'\rangle = \delta_{x,x'}$ - the Kronecker δ . Taking expectation value of the second equation above, it follows that $\beta f(x, \beta) = 0, \forall x, \beta \in \mathbb{R}$, where $f(x, \beta) := \langle x|\hat{W}(i\beta/\sqrt{2})|x\rangle$. This implies that $f(x, \beta)$ is zero for $\beta \neq 0$ and $f(x, 0) = 1$ directly from the definition. Thus $f(x, \beta)$ cannot be continuous at $\beta = 0$, for any x . This means $\hat{W}(i\beta/\sqrt{2})$ cannot be weakly continuous at $\beta = 0$.

This also means that if $\hat{W}(i\beta/\sqrt{2})$ is weakly continuous (as for the Schrodinger representation), then \hat{X} cannot have any eigenvector. Each $x \in \mathbb{R}$ is a generalised eigenvalue and hence, in the formal notation, $\langle x|x'\rangle = \delta(x - x')$ - the Dirac δ -function.

Thus, in the Schrodinger representation, \hat{X} necessarily has only generalised eigenvalues, while in the polymer representation, it could have proper eigenvalues, but generalized eigenvalues is not ruled out.

However, in the polymer representation, we note:

$$\langle W(i\beta/\sqrt{2}), W(i\beta'/\sqrt{2}) \rangle = \Omega_{\text{Poly}} \left(W(-i\beta/\sqrt{2})W(i\beta'/\sqrt{2}) \right) = \delta_{\beta,\beta'} ; \quad (5.26)$$

$$\langle W(i\beta/\sqrt{2}), \hat{X} \{ W(i\beta'/\sqrt{2}) \} \rangle = -\beta\delta_{\beta,\beta'} \quad (5.27)$$

$$\begin{aligned} \left\| (\hat{X} - \lambda\mathbb{I})[W(i\beta/\sqrt{2})] \right\| &= \lim_{\alpha \rightarrow 0} \left\| \frac{1}{i\alpha} \left[W\left(\frac{\alpha+i\beta}{\sqrt{2}}\right) - (1 + i\alpha\lambda) \right] W(i\beta/\sqrt{2}) \right\| \\ &= 0 \quad \text{for } \lambda = -\beta . \end{aligned} \quad (5.28)$$

which show explicitly that $W(-i\beta/\sqrt{2})$ is a normalized eigenvector of \hat{X} with eigenvalue β , for every $\beta \in \mathbb{R}$. This means that the Polymer Hilbert space is *non-separable*.

This concludes the illustration of the GNS construction of representations of C^* algebras. In the next sub-section we see the analogue of the spin network construction.

5.2.4 Polymer representation via ‘spin networks’

We begin by introducing ‘graphs’ in a ‘0-dimensional manifold’, define ‘holonomies’ and ‘spin network functions’, define an inner product and densely defined operators. More details may be seen in [24].

1. *Graphs, holonomies, cylindrical functions:* Any countable set of real numbers, $\{x_i\}$ represents a *graph* and is denoted by γ^5 . Note that the ‘points’ x_j on the real line correspond to *edges*. Associated to each edge, x_j , we define a *point holonomy*, e^{ikx_j} , $k \in \mathbb{R}$ plays the role of a *connection*. For each graph γ , define complex valued functions, $f_\gamma(k) := \sum_j f_j e^{ikx_j}$. Let Cyl_γ denote the vector space of $f_\gamma(k)$. Elements of this vector space are said to be *functions cylindrical with respect to the graph* γ . Let $\text{Cyl} := \sum_{\oplus} \text{Cyl}_\gamma$, where the sum is over all possible graphs.

Thus a general element of Cyl is a function of k expressible as a countable linear combination of the *elementary functions* $f_{x_j}(k) := e^{ikx_j}$'s.

⁵For precise technical conditions, please refer to [24]

2. *Inner Product on Cyl*: Define

$$\langle f, g \rangle_{\text{Poly}} := \lim_{L \rightarrow \infty} \frac{1}{2L} \int_{-L}^L dk f^*(k) g(k)$$

which for elementary functions $f_{x_j}(k), f_{x_l}(k)$ gives δ_{x_j, x_l} . Introducing the notation, $|x_j\rangle \leftrightarrow e^{ikx_j}$ this is expressed as $\langle x_j, x_l \rangle := \delta_{x_j, x_l}, \forall x_j, x_l \in \mathbb{R}$. Cauchy completion of Cyl with respect to this inner product defines a Hilbert space, $\mathcal{H}_{\text{Poly}}$.

3. *Action of \mathcal{W}* : Define operators $\hat{W}(z)$ on Cyl by,

$$\hat{W}\left(\frac{\alpha+i\beta}{\sqrt{2}}\right) f(k) := e^{-i\alpha\beta/2} e^{i\beta k} f(k - \alpha) \quad , \quad \forall f \in \text{Cyl}, \forall \alpha, \beta \in \mathbb{R}$$

These are densely defined and can be extended to bounded unitary operators on $\mathcal{H}_{\text{Poly}}$. It is easily verified that this provides a representation of the abstract algebra defined in (5.13).

Exercise: Show that the 1-parameter families of unitary operators, $\hat{W}(\alpha/\sqrt{2})$ and $\hat{W}(i\beta/\sqrt{2})$ are weakly continuous at $\alpha = 0$ and weakly discontinuous at $\beta = 0$ respectively. This implies that while \hat{X} can be defined from the $\hat{W}(\alpha/\sqrt{2})$ family, there is no corresponding operator from the second family. Thus the holonomies - $h_{x_j}(k)$ are well defined but not the connection - k itself.

5.2.5 Harmonic Oscillator in the polymer representation

So we see two distinct representations of the same abstract algebra with the polymer representation being similar to the LQG representation. Are there observable quantities which would reveal which representation occurs in nature?

An obvious candidate is to consider the dynamics of the Harmonic oscillator, with the classical Hamiltonian, $H(x, p) := p^2/(2m) + m\omega^2 x^2/2, \{x, p\} = 1$. In the quantum theory, the x, p are expected to be replaced by the corresponding operators. However, in the polymer representation, there is no \hat{p} ! So in proposing the quantum Hamiltonian we need to introduce a *scale*, μ_0 and *define* $\hat{p}^2 := \{2 - \hat{W}(i\mu_0/\sqrt{2}) + \hat{W}(-i\mu_0/\sqrt{2})\}/\mu_0^2$. We could of course define \hat{p} first and then take its square. This is a quantization ambiguity not too important for our purposes here [24]. In the Schrodinger representation, we could use exactly the same definition, work out quantities of interest eg spectrum and then take the limit $\mu_0 \rightarrow 0$. In the polymer representation, we *cannot* take this limit.

Consider the eigenvalue equation for the Hamiltonian: $\hat{H}|\psi\rangle = E|\psi\rangle$. Writing $|\psi\rangle := \sum_{x \in \text{countable set}} \psi(x)|x\rangle$, and noting that the unitary operators in \hat{p}^2 shift the $|x\rangle \rightarrow |x \pm \mu_0\rangle$, the eigenvalue equation becomes a *difference* equation, involving $\psi(x), \psi(x \pm \mu_0)$. This means that $\psi(x)$ with x in a lattice $L_{x_0} := \{x = x_0 + \mu_0 N, N \in \mathbb{Z}\}$ constitute a solution while those belonging to different lattices are unrelated. Span of the vectors in any lattice form a *separable* subspace of the polymer Hilbert space. The spectrum can be determined for each lattice independently. This is analyzed in detail in [24]. Suffice it to say that the spectrum differs from that in the Schrodinger representation by terms down by powers of μ_0/d . Here, $d := \sqrt{\hbar/m\omega}$ is the length scale defined by the system while μ_0 is the length scale introduced by the approximation for the momentum operator. For the physical systems modelled well

by an oscillator (eg for vibrational spectra of molecules), μ_0/d is extremely small and so Schrodinger vs polymer representation cannot be resolved by observations.

Additional comments may be seen in [24].

5.3 Inverse Triad Operator(s)

As noted before, the discrete nature of the spectrum of the triad operator implies that its inverse is not densely defined. Consequently the counterpart of the classical function p^{-1} needs to be defined indirectly, by a suitable prescription. Being a prescription, it introduces quantization ambiguities. We will consider a prescription which is sufficiently general.

We aim to define an operator $\widehat{\text{sgn}(p)}|p|^{-1}$. Introduce the following notation: n^i is a unit, 3-dimensional vector and τ_i are anti-hermitian generators of $SU(2)$ in the J^{th} representation, satisfying

$$[\tau_i, \tau_j] = \epsilon_{ijk}\tau_k \quad , \quad \text{Tr}_J(\tau_i\tau_j) = -\frac{1}{3}J(J+1)(2J+1)\delta_{ij} \quad := \quad -\mathcal{N}_J\delta_{ij}$$

For $f_\alpha(p) := \mu_\alpha|p|^{-\alpha/2}$, and define $g_\alpha(p) := \int^p f_\alpha^{-1}(x)dx = \mu_\alpha^{-1}\widehat{\text{sgn}(p)}|p|^{1+\alpha/2}(1+\alpha/2)^{-1}$. For $\alpha = 0$ we have $f_0 = \mu_0$ while for $\alpha = 1$ we have $f_1 = \mu_1|p|^{-1/2}$ and we choose $\mu_1 := \ell_P\sqrt{\gamma\sqrt{3}/4}$. These recover the μ_0 and the $\bar{\mu}$ schemes. We will suppress the α label. Define $h_f := e^{\lambda n^i \tau_i f(\alpha,p)c}$. This is matrix of order $(2J+1)$. Classically, the following is true.

$$h_f\{h_f^{-1}, |g|^l(p)\} = -\frac{\kappa\gamma}{3}(\lambda n^i \tau_i) l|g|^{l-1}\widehat{\text{sgn}(p)} \text{ where we used } f\frac{d|g|}{dp} = \widehat{\text{sgn}(p)}. \quad (5.29)$$

$$|p|^{(l-1)(1+\alpha/2)} = \widehat{\text{sgn}(p)} \left[\frac{3}{\kappa\gamma l \lambda} (\mu_\alpha(1+\alpha/2))^{l-1} \mathcal{N}_J^{-1} \right] \times [\text{Tr}_J((n^i \tau_i) h_f\{h_f^{-1}, |g|^l\})] \quad (5.30)$$

$$= \widehat{\text{sgn}(p)} \left[\frac{\kappa\gamma l \lambda}{3} (\mu_\alpha(1+\alpha/2)) \mathcal{N}_J \right]^{-1} \times [\text{Tr}_J((n^i \tau_i) h_f\{h_f^{-1}, |p|^{l(1+\alpha/2)}\})] \quad (5.31)$$

Thus we have a classical expression for $|p|^{(l-1)(1+\alpha/2)}$ which has *four* ambiguity parameters: α, J, l, λ . J is a positive half integer, $0 < l < 1, \alpha > -2$. The special cases would be: (a) μ_0 -scheme: $\alpha = 0, \lambda = 1$; (b) improved scheme: $\alpha = 1, \lambda = 1, j = 1/2$ and some special values of l explored; (c) Madhavan scheme: similar to the improved scheme except λ is correlated with the fiducial volume V_0 (more on this later). We could *choose* $l-1 = (1+\alpha/2)^{-1}$ to define inverse triad, but we will postpone such choices.

The corresponding quantum operator is obtained by replacing the Poisson bracket by $-i\hbar^{-1}$ times the commutator. The $-i$ is combined with $n \cdot \tau$ to make the generators Hermitian and the \hbar^{-1} combines with κ to replace κ by ℓ_P^2 . The commutator is expanded as: $\hat{h}_f[\hat{h}_f^{-1}, \widehat{|g|^l}] = \text{I.} \widehat{|g|^l} - \hat{h}_f \widehat{|g|^l} \hat{h}_f^{-1}$.

Observe that $n \cdot (-i\tau)$ can be diagonalised with diagonal elements being $-J, -J+1, \dots, J-1, J$. So the h_f becomes the diagonal matrix $e^{(i\lambda f_\alpha c)(J, J-1, \dots, -J+1, -J)}$. So the commutator terms are diagonal matrices.

The computations simplify if we label the basis states by ⁶

$$v_\alpha := \left(\frac{1}{6}\gamma\ell_P^2\right)^{\alpha/2} \left(\frac{1}{\mu_\alpha(1+\alpha/2)}\right) \text{sgn}(\mu)|\mu|^{1+\alpha/2}, \quad \hat{g}_\alpha|v_\alpha\rangle = \frac{\gamma\ell_P^2}{6}v_\alpha|v_\alpha\rangle \quad (5.32)$$

So that the h_f shifts the v_α labels simply as,

$$\widehat{e^{i\lambda k f_\alpha c}}|v_\alpha\rangle = |v_\alpha + 2k\lambda\rangle \quad \because \quad e^{ifc/2}|v\rangle = |v+1\rangle.$$

With these, acting on a basis state $|v_\alpha\rangle$, the Tr_J evaluates to,

$$\begin{aligned} [\text{Tr}_J\{\dots\}] &= \left(\frac{\gamma\ell_P^2}{6}\right)^l \sum_{k=-J}^J k \{|v_\alpha|^l - |v_\alpha - 2k\lambda|^l\} \\ &= \left(\frac{\gamma\ell_P^2}{6}\right)^l \sum_{k=-J}^J k|v_\alpha + 2k\lambda|^l \quad \text{and defining } v_\alpha := 2J\lambda q_\alpha, \\ &= \left(\frac{\gamma\ell_P^2\lambda}{6}\right)^l 2^l \sum_{k=-J}^J k|Jq_\alpha + k|^l := \left(\frac{\gamma\ell_P^2\lambda}{3}\right)^l \text{sgn}(q_\alpha)G_{J,l}(q_\alpha) \end{aligned} \quad (5.33)$$

$$G_{J,l}(q_\alpha) := \text{sgn}(q_\alpha) \sum_{k=-J}^J k|Jq_\alpha + k|^l \quad (5.34)$$

The eigenvalues of $|p|^{\widehat{(l-1)(1+\alpha/2)}}$ are then given by

$$\begin{aligned} |p|^{\widehat{(l-1)(1+\alpha/2)}}|v_\alpha\rangle &:= \text{sgn}(v_\alpha)\Lambda_{J,l,\alpha}(v_\alpha)|v_\alpha\rangle \\ \Lambda_{J,l,\alpha}(v_\alpha) &= \left(\frac{\mu_\alpha\gamma\ell_P^2\lambda}{3}\right)^{l-1} \frac{(1+\alpha/2)^{l-1}}{l} \mathcal{N}_J^{-1}[G_{J,l}(q_\alpha)] \end{aligned} \quad (5.35)$$

The first bracket takes care of the dimensions and the remaining factors are dimensionless. It remains to calculate the last square bracket which is a λ, α independent, universal function of its argument and depends only on J, l .

From its definition, it is easy to see that $G_{J,l}(0) = 0$ and $G_{J,l}(-q_\alpha) = G_{J,l}(q_\alpha)$, the $\text{sgn}(q_\alpha)$ factor is crucial for this. Thus it suffices to consider only $q_\alpha > 0$.

$$\begin{aligned} G_{j,l}(q_\alpha > 0) &= \sum_{k=-J}^J k|k + Jq_\alpha|^l \\ &= \sum_{k=-J}^J \{(k + Jq_\alpha)|k + Jq_\alpha|^l - Jq_\alpha|k + Jq_\alpha|^l\} \\ &= \sum_{k=J(q_\alpha-1)}^{J(q_\alpha+1)} \{\text{sgn}(k)|k|^{l+1} - Jq_\alpha|k|^l\} \end{aligned} \quad (5.36)$$

$$G_{j,l}(q_\alpha \geq 1) = \sum_{k=J(q_\alpha-1)}^{J(q_\alpha+1)} \{|k|^{l+1} - Jq_\alpha|k|^l\} \quad (5.37)$$

$$G_{j,l}(0 < q_\alpha < 1) = - \sum_{k=J(q_\alpha-1)}^{0_-} \{|k|^{l+1} + Jq_\alpha|k|^l\} + \sum_{0_+}^{k=J(q_\alpha+1)} \{|k|^{l+1} - Jq_\alpha|k|^l\} \quad (5.38)$$

⁶The functions $f_\alpha(p)$ are taken to be dimensionless. This makes the μ_α to have dimensions of ℓ_P^α and $g_\alpha(p)$ to have dimensions of ℓ_P^2 . The v_α is defined to be dimensionless.

In the second step, we have shifted $k \rightarrow k - Jq_\alpha$. k is no longer integral but still changes in steps of 1. Clearly, for $q_\alpha \geq 1$, k is positive and the sgn as well as the absolute value are redundant (the $k = 0$ term for $q_\alpha = 1$ gives zero and hence the sum is confined to positive k only), as in (5.37). For $q_\alpha < 1$, the sum splits in two groups as in (5.38), and the 0_\pm denote the respective limits on the values of k which must match with the other limits and shift in steps of 1.

We will not simplify/approximate this further but consider the special cases (i) $\alpha = 0, \lambda = 1$ and (ii) $\alpha = 1, J = 1/2, l = 2/3$.

(i) $\alpha = 0, \lambda = 1$: (eigenvalues of $|p|^{l-1}$)

$$f_0(p) = \mu_0 \quad , \quad g_0(p) = \mu_0^{-1} \text{sgn}(p)|p| \quad , \quad V_0 = \mu_0^{-1} \text{sgn}(\mu)|\mu| \quad (5.39)$$

$$\Lambda_{J,l,0}(V_0) = \left(\frac{\mu_0 \gamma \ell_P^2}{3} \right)^{l-1} (l\mathcal{N}_J)^{-1} G_{J,l}(|\mu|/(2J\mu_0)) \quad (5.40)$$

$$\Lambda_{\frac{1}{2}, \frac{1}{2}, 0}(V_0) = \left(\frac{\gamma \ell_P^2}{6} \right)^{-1/2} \frac{1}{\sqrt{\mu_0}} \left(\left| \frac{\mu}{\mu_0} + 1 \right|^{1/2} - \left| \frac{\mu}{\mu_0} - 1 \right|^{1/2} \right) \quad (5.41)$$

(ii) $\alpha = 1, J = 1/2$: (eigenvalues of $|p|^{\frac{3}{2}(l-1)}$)

$$f_1(p) = \mu_1 |\mu|^{-1/2} \quad , \quad \mu_1 := \sqrt{\frac{\gamma \ell_P^2}{6} \frac{3\sqrt{3}}{2}} \quad , \quad g_0(p) = \mu_1^{-1} \text{sgn}(p)|p|^{3/2} (3/2)^{-1} \quad , \quad (5.42)$$

$$v_1 = \left(\frac{\gamma \ell_P^2}{6} \right)^{1/2} \mu_1^{-1} (3/2)^{-1} \text{sgn}(\mu) |\mu|^{3/2} = K \text{sgn}(\mu) |\mu|^{3/2} \quad (5.43)$$

$$\Lambda_{\frac{1}{2}, l, 1}(v_1) = \left(\frac{\mu_1 \gamma \ell_P^2}{3} \frac{3}{2} \lambda \right)^{l-1} (l\mathcal{N}_{\frac{1}{2}})^{-1} G_{1/2, l}(|v_1|/(2\frac{1}{2}\lambda)) \quad (5.44)$$

The G can be computed directly from the (5.34), for $v_1 > 0$, as

$$G_{\frac{1}{2}, l}(v_1/\lambda) = \left(\frac{1}{2} \right)^{l+1} \left(\left| \frac{v_1}{\lambda} + 1 \right|^l - \left| \frac{v_1}{\lambda} - 1 \right|^l \right) \quad (5.45)$$

For $l = 2/3$ the operator becomes $|p|^{-1/2}$ and the eigenvalue becomes,

$$\Lambda_{\frac{1}{2}, \frac{2}{3}, 1}(v_1) = \left(\frac{\gamma \ell_P^2}{6} \right)^{-1/2} \frac{3}{4} \left(\frac{K}{\lambda} \right)^{\frac{1}{3}} \left[\left| \frac{v_1}{\lambda} + 1 \right|^{\frac{2}{3}} - \left| \frac{v_1}{\lambda} - 1 \right|^{\frac{2}{3}} \right] \quad (5.46)$$

For large v_1 and $\lambda = 1$, this matches with the eigenvalue given by [20]⁷. The difference arises because the APS prescription takes the $\alpha = 0$ expression and replaces μ_0 by $\bar{\mu}$ in equation (5.31).

For large J the sum can be approximated using,

$$\int_0^1 dx x^r = \frac{1}{r+1} \approx \sum_{i=1}^N \left(\frac{i}{N} \right)^r \frac{1}{N} \Rightarrow \sum_{i=1}^N i^r \approx \frac{N^{r+1}}{(r+1)}$$

and applying it to the sums in the definition of the $G_{J,l}$.

⁷Actually, for large volume, the leading term is *independent* of λ . The sub-leading (correction) terms, do depend on λ .

5.4 Inhomogeneous Lattice Models

In the main body, we focused on quantization of *symmetry reduced models* which are based on a homogeneous and isotropic background. From a perspective of the full theory, this background presumably corresponds to a state of full theory. Generic states of the full theory would be inhomogeneous. One way in which symmetric states of the full theory have been understood in the LQC context is that the symmetric states are those distributions in Cyl^* of the full theory which have support on the invariant connections [23]. In the same spirit, we may stipulate certain kinds of inhomogeneous states as those distributions which have support on certain form of ‘inhomogeneous connections’. Specific models can be then constructed using similar strategies as used in LQC constructions. Such models can shed some light on how homogeneous and isotropic models could be viewed from an inhomogeneous perspective. These so-called lattices models are briefly summarised below. Details should be seen in [16].

For definiteness, let us continue to work with homogeneous (not necessarily isotropic), spatially flat, diagonalised model with a fiducial cell of co-moving volume V_0 as before. The spatial isometries provide directions (of the Killing vectors) and the fiducial metric provides coordinates as background structures which are to be kept fixed. Using these background structures, Bojowald constructs another model as follows.

Choose a cubical lattice (say) aligned with the isometry directions and with a spacing $\ell_0 := (V_0/N)^{1/3}$. Let the vertices of the lattices be denoted by \vec{v} and the three oriented links be denoted by $\vec{e}_{I,\vec{v}}(t) := \vec{v} + t\hat{e}_I$, $t \in [0, \ell_0]$ and \hat{e}_I is the unit vector in the I^{th} direction. For future reference, let $S_{I,\vec{v}}$ denote the elementary surface perpendicular to the elementary link $\vec{e}_{I,\vec{v}}$ and passing through its mid-point.

Restrict the connections and triad variables to be of the form,

$$A_a^i(x) := \tilde{k}_I(x)\delta_{(I)}^i\delta_a^I, \quad E_i^a(x) := \tilde{p}^I(x)\delta_i^{(I)}\delta_I^a. \quad (5.47)$$

These are the local versions of the diagonalised homogeneous models. The diagonal form of the connections implies that the holonomies - path ordered exponentials - become ordinary exponentials of line integrals.

The \tilde{k}_I, \tilde{p}^I are further taken to be spatially periodic with period $V_0^{1/3}$,

$$\tilde{k}_I(x) = \sum_{\vec{m}} \tilde{k}_I(\vec{m})e^{i\vec{m}\cdot\vec{x}}, \quad \tilde{p}^I(x) = \sum_{\vec{m}} \tilde{p}^I(\vec{m})e^{i\vec{m}\cdot\vec{x}}, \quad \vec{m} = 2\pi V_0^{-1/3}\vec{n}, \quad \vec{n} \in \mathbb{Z}^3. \quad (5.48)$$

The Poisson brackets between the connection and the triad lead to,

$$\{\tilde{k}_I(x), \tilde{p}^J(y)\} = \kappa\gamma\delta_I^J\delta^3(x, y). \quad \Rightarrow \quad \{\tilde{k}_I(\vec{m}), \tilde{p}^J(\vec{m}')\} = \kappa\gamma V_0^{-1}\delta_I^J\delta^3(\vec{m}, -\vec{m}'). \quad (5.49)$$

In loop quantization, basic variables of the model will be holonomies of the lattice connection along the three elementary links at each vertex and the three fluxes of the lattice triad variables along the elementary surfaces through the mid-points of the elementary links and perpendicular to the link. As noted above, these holonomies will be ordinary exponentials thanks to the diagonal form of the connection.

The line integrals of the connection along elementary links of the lattice are given by,

$$\begin{aligned} \mathcal{I}_{I,\vec{v}} &:= \int_{\vec{e}_{I,\vec{v}}} dt \tilde{k}_I(\vec{e}_I(t)) = \int_{\vec{e}_{I,\vec{v}}} dt \sum_{\vec{m}} \tilde{k}_I(\vec{m}) e^{i\vec{m}\cdot\vec{e}_{I,\vec{v}}(t)} = \sum_{\vec{m}} \tilde{k}_I(\vec{m}) e^{i\vec{m}\cdot\vec{v}} \int_0^{\ell_0} dt e^{it\vec{m}\cdot\hat{e}_I} \\ &= \sum_{\vec{m}} \tilde{k}_I(\vec{m}) \left\{ 2 e^{i\vec{m}\cdot\vec{v}} e^{im_I\ell_0/2} \left(\frac{\sin(m_I\ell_0/2)}{m_I} \right) \right\} \quad \text{where, } m_I := \vec{m} \cdot \hat{e}_I . \end{aligned} \quad (5.50)$$

$$\approx \tilde{k}_I(\vec{v})\ell_0 \quad \because \quad m_I\ell_0 \ll 1 \text{ dominates the sum.}$$

$$h_{I,\vec{v}} := e^{\frac{i}{2}\mathcal{I}_{I,\vec{v}}} \approx e^{\frac{i}{2}\tilde{k}_I(\vec{v})\ell_0} := e^{\frac{i}{2}k_I(\vec{v})} \quad (\text{elementary holonomies}) \quad (5.51)$$

Likewise, the fluxes of the lattice triad along elementary surfaces are given by,

$$\begin{aligned} \mathcal{F}_{\vec{v}}^J &:= \int_{S_{J,\vec{v}}} \sum_{\vec{m}} \tilde{p}^J(\vec{m}) e^{\vec{m}\cdot\vec{y}} = \sum_{\vec{m}} \tilde{p}^J(\vec{m}) e^{\vec{m}\cdot\vec{v}} e^{im_J\ell_0/2} \int_{-\ell_0/2}^{\ell_0/2} e^{itm_K} dt \int_{-\ell_0/2}^{\ell_0/2} e^{itm_L} dt \\ &= \sum_{\vec{m}} \tilde{p}^J(\vec{m}) \left\{ 4e^{i\vec{m}\cdot\vec{v}} e^{im_J\ell_0/2} \left(\frac{\sin(m_K\ell_0/2)\sin(m_L\ell_0/2)}{m_K m_L} \right) \right\} \end{aligned} \quad (5.52)$$

$$\approx \tilde{p}_I(\vec{v})\ell_0^2 \quad (\text{elementary fluxes}) \quad (5.53)$$

The J, K, L indices are chosen such that $\epsilon_{JKL} = 1$. This takes care of the orientations. There are no smearing functions above because the \tilde{p}^I variables are (U(1)) gauge invariant thanks to diagonalised form.

These variables satisfy the Poisson brackets,

$$\begin{aligned} \{\mathcal{I}_{I,\vec{v}}, \mathcal{F}_{\vec{v}'}^J\} &= \kappa\gamma\delta_I^J \left[8V_0^{-1} \sum_{\vec{m}} e^{i\vec{m}\cdot(\vec{v}-\vec{v}')} \frac{\sin(m_I\ell_0/2)\sin(m_K\ell_0/2)\sin(m_L\ell_0/2)}{m_I m_K m_L} \right] \\ &= \kappa\gamma\delta_I^J [\chi_{\ell_0}(\vec{v}-\vec{v}')] = \kappa\gamma\delta_I^J \delta_{\vec{v},\vec{v}'} \end{aligned} \quad (5.54)$$

The square brackets above is the characteristic function of width ℓ_0 and centered at $(\vec{v}-\vec{v}')$ which is just the Kronecker delta.

The kinematical Hilbert space is then described in terms of the flux representation as:

$$\hat{\mathcal{F}}_{\vec{v}}^I |\dots, \mu_{I,\vec{v}}, \dots\rangle = \left(\frac{\gamma\ell_P^2}{2} \mu_{I,\vec{v}} \right) |\dots, \mu_{I,\vec{v}}, \dots\rangle \quad , \quad \mu_{I,\vec{v}} \in \mathbb{Z} \quad (5.55)$$

$$\hat{h}_{I,\vec{v}} |\dots, \mu_{I,\vec{v}}, \dots\rangle = |\dots, \mu_{I,\vec{v}} + 1, \dots\rangle \quad (5.56)$$

The flux eigenvalues are in *integer* steps of $\gamma\ell_P^2/2$ because the elementary holonomies suffice to separate the *lattice connections* (periodic) and thus only their integer powers appear.

Subsequent steps are similar to what is done in the homogeneous models. In particular, the volume corresponding to the cell with N^3 lattice sites, can be expressed as

$$\begin{aligned} V &= \int d^3x \sqrt{|\tilde{p}^1\tilde{p}^2\tilde{p}^3|} \approx \sum_{\vec{v}} \ell_0^3 \sqrt{|\tilde{p}^1(\vec{v})\tilde{p}^2(\vec{v})\tilde{p}^3(\vec{v})|} = \sum_{\vec{v}} \sqrt{|p^1(\vec{v})p^2(\vec{v})p^3(\vec{v})|} \\ &\approx \sum_{\vec{v}} \sqrt{|\mathcal{F}_{\vec{v}}^1\mathcal{F}_{\vec{v}}^2\mathcal{F}_{\vec{v}}^3|} \end{aligned} \quad (5.57)$$

leading to the corresponding operator expression.

There is no diffeomorphism constraint since the background coordinates are fixed in defining the lattice, the SU(2) gauge invariance is first reduced to the U(1)³ due to restriction to diagonal connection and triad and by the form of these variables, the \tilde{k}_I, \tilde{p}^I are gauge invariant variables. Hamiltonian constraint remains as in the case of homogeneous models. In essence, we have N^3 ‘homogeneous models’ (labelled by the Fourier label \vec{m}) at the level of basic variables and the kinematical Hilbert space. The role that V_0 played in the homogeneous model is now played by ℓ_0 . The *inhomogeneity* is reflected by basis states having *different values* of $\mu_{I,\vec{v}}$ variables.

How do we relate this set-up to the isotropic one discussed before?

Observe that a generic basis state in the lattice model will be,

$$\psi_{\{\mu_{I,\vec{v}}\}}[h_{I,\vec{v}}] = \prod_{I,\vec{v}} (h_{I,\vec{v}})^{\mu_{I,\vec{v}}} := \langle k_J(x) | \dots, \mu_{I,\vec{v}}, \dots \rangle \quad , \quad k_J(x) := \tilde{k}_J(x) \ell_0 . \quad (5.58)$$

If we choose $\tilde{k}(x) := \tilde{c} := V_0^{-1/3} c \forall x, I$, then the basis function becomes a function of a single variable c (which is independent of x), and is of the form:

$$\psi_\mu(c) = e^{i\mu c/2} \quad , \quad \mu := N^{-1/3} \sum_{I,\vec{v}} \mu_{I,\vec{v}} \in \mathbb{Q} ; \quad (5.59)$$

which can be viewed as a basis element of $\text{Cyl}_{\text{isotropic}}$. Thus we can define a map $\pi : \text{Cyl}_{\text{lattice}} \rightarrow \text{Cyl}_{\text{isotropic}}$,

$$\begin{aligned} \pi : | \dots, \mu_{I,\vec{v}}, \dots \rangle &\rightarrow |\mu\rangle \Leftrightarrow \langle c|\mu\rangle := \langle k_J(x) | \dots, \mu_{I,\vec{v}}, \dots \rangle |_{\tilde{k}(x)=\tilde{c}} \\ &\text{with } \mu := N^{-1/3} \sum_{I,\vec{v}} \mu_{I,\vec{v}} \end{aligned} \quad (5.60)$$

Note that the image of π -map is a separable subspace of $\text{Cyl}_{\text{isotropic}}$, spanned by $|\mu\rangle, \mu \in \mathbb{Q}$.

Clearly we cannot *uniquely* identify a cylindrical state of the lattice model, given a cylindrical state of the isotropic model. However, we can define a map $\sigma : \text{Cyl}_{\text{isotropic}} \rightarrow \text{Cyl}_{\text{lattice}}^*$, $\sigma : |\mu\rangle \rightarrow (\mu|, \mu \in \mathbb{R}$, such that,

$$(\mu| \dots, \nu_{I,\vec{v}}, \dots) = \langle \mu | \pi(| \dots, \nu_{I,\vec{v}}, \dots) \rangle = \delta_{\mu,\nu} \quad , \quad \nu := N^{-1/3} \sum_{I,\vec{v}} \nu_{I,\vec{v}} . \quad (5.61)$$

In the second equality, we have used the inner product of the isotropic model. This map embeds cylindrical states of the isotropic model into the distributional states of the lattice model⁸.

Now, we have Operators A^* acting on $\text{Cyl}_{\text{lattice}}^*$ corresponding to operators A acting on the $\text{Cyl}_{\text{lattice}}$, defined in the usual manner. Those of these operators which act *invariantly* on the image of σ in $\text{Cyl}_{\text{lattice}}^*$, can be identified with operators of the isotropic model. For these operators, we can define $A_{\text{isotropic}}$ via the equation: $\sigma(A_{\text{isotropic}}|\mu\rangle) := (\sigma|\mu\rangle)A_{\text{lattice}}^*$. Since we have embedded isotropic states in the distributions of the lattice model and also have correspondence between operators, matrix elements computed in the isotropic model can be understood as actions of lattice distributions on lattice cylindrical states.

⁸Notice that μ, ν defined above are *rationals with a common denominator* $N^{1/3}$. Therefore the distributions $(\mu|$ are non-trivial only for $\mu \in \mathbb{Q}$ with the same denominator.

Consider an operator A_{lattice} on $\text{Cyl}_{\text{lattice}}$. This defines an operator A_{lattice}^* on $\text{Cyl}_{\text{lattice}}^*$: $(A_{\text{lattice}}^* \phi | \dots, \nu_{I, \vec{v}}, \dots) := (\phi | \{A_{\text{lattice}} | \dots, \nu_{I, \vec{v}}, \dots\})$. If, for every distribution $(\phi | = (\mu | =: \sigma(|\mu))$, the operator A_{lattice}^* gives another distribution $(\mu' | =: \sigma|\mu')$, then we get an operator on $\text{Cyl}_{\text{isotropic}}$: $A_{\text{isotropic}}|\mu\rangle := |\mu'\rangle$.

It is easy to see that the multiplicative operators on $\text{Cyl}_{\text{lattice}}$, give multiplicative operators on $\text{Cyl}_{\text{isotropic}}$. For example, taking $A_{\text{lattice}} = h_{J, \vec{v}}$, the lattice state $|\dots, \nu_{I, \vec{v}}, \dots\rangle$ will have the $\nu_{J, \vec{v}}$ incremented by 1. The action of the $(\mu |$ will give $\delta_{\mu, \nu+1}$. This can be understood as the action of $(\mu - 1 |$ on the original lattice state. Thus $(A_{\text{lattice}}^* \mu | = (\mu - 1 |$ which implies the a multiplicative action $A_{\text{isotropic}}|\mu\rangle := |\mu - 1\rangle$.

For elementary flux operators, little more work is needed. For example, action of $\hat{\mathcal{F}}_{\vec{v}}^I$ on a basis state, $|\dots, \nu_{J, \vec{v}}, \dots\rangle$ is zero unless $\nu_{J, \vec{v}} \neq 0$ for some $J = I$ and at some $\vec{v}' = \vec{v}$ i.e.

$$\begin{aligned} \hat{\mathcal{F}}_{\vec{v}}^I |\nu_{J, \vec{v}}\rangle &= \frac{1}{2} \gamma \ell_{\text{P}}^2 \nu_{J, \vec{v}} \delta_J^I \delta_{\vec{v}, \vec{v}'} |\nu_{J, \vec{v}}\rangle \quad \text{or} \\ (\mu | \hat{\mathcal{F}}_{\vec{v}}^I |\nu_{J, \vec{v}}\rangle &= \left[\frac{1}{2} \gamma \ell_{\text{P}}^2 \nu_{J, \vec{v}} \right] \delta_J^I \delta_{\vec{v}, \vec{v}'} \delta_{\mu, \nu} \quad , \quad \nu := N^{-1/3} \nu_{J, \vec{v}} \quad \text{However,} \quad (5.62) \\ (\mu' | \nu_{I, \vec{v}'}\rangle &= (\mu' | \nu_{I, \vec{v}''}\rangle \quad \forall \quad (\mu' |, \vec{v}', \vec{v}'' \quad . \quad (5.63) \end{aligned}$$

Thus $(\hat{\mathcal{F}}_{\vec{v}}^I)^*$ cannot act invariantly on the image of σ in $\text{Cyl}_{\text{lattice}}^*$. It is clear though that if we *sum* the elementary flux operators (with the directional index I) over *all* the lattice sites (this is a finite sum due to the cell), then the sum will act invariantly. By averaging over the directions as well, we can construct an operator corresponding to a ‘flux’ operator on $\text{Cyl}_{\text{isotropic}}$. In equations,

$$\begin{aligned} \hat{p}_{\text{lattice}}^I &:= N^{-1/3} \sum_{\vec{v}} \hat{\mathcal{F}}_{\vec{v}}^I \quad , \quad \hat{p}_{\text{lattice}} := \frac{1}{3} \sum_I \hat{p}_{\text{lattice}}^I \quad \Rightarrow \quad (5.64) \\ (\mu | \{\hat{p}_{\text{lattice}} | \dots, \nu_{J, \vec{v}}, \dots\} &= \frac{1}{6} \gamma \ell_{\text{P}}^2 N^{-1/3} \sum_{J, \vec{v}} \nu_{J, \vec{v}} (\mu | \dots, \nu_{J, \vec{v}}, \dots) \\ &= \frac{1}{6} \gamma \ell_{\text{P}}^2 \nu \delta_{\mu, \nu} \quad , \quad \nu := N^{-1/3} \sum_{I, \vec{v}} \nu_{J, \vec{v}} \quad (5.65) \end{aligned}$$

The last expression is exactly the matrix element of the \hat{p} operator defined in the isotropic model. As noted in the footnote, the identification of the matrix elements is restricted to $\mu, \nu \in \mathbb{Q}$.

This completes our summary of the lattice model and how isotropic model is ‘embedded’ in the lattice model. This ‘embedding’ refers to embedding of the particular separable subspace of $\text{Cyl}_{\text{isotropic}}$.

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