Time in quantum cosmology

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Abstract

A cosmological model with two global internal times shows that time reparameterization invariance, and therefore covariance, is not guaranteed by deparameterization. In particular, it is impossible to derive proper-time effective equations from a single deparameterized model if quantum corrections from fluctuations and higher moments are included. The framework of effective constraints shows how proper-time evolution can consistently be defined in quantum cosmological systems, such that it is time reparameterization invariant when compared with other choices of coordinate time. At the same time, it allows transformations of moment corrections in different deparameterizations of the same model, indicating partial time reparameterization of internal-time evolution. However, in addition to corrections from moments such as quantum fluctuations, also factor ordering corrections may appear. The latter generically break covariance in internal-time formulations. Fluctuation effects in quantum cosmology are therefore problematic, in particular if derivations are made with a single choice of internal time or a fixed physical Hilbert space.

1 Introduction

Deparameterization has become a popular method to circumvent the problem of time in canonical quantum gravity. Since coordinate time is observer-dependent and does not have a corresponding operator after quantization, one instead selects one of the phase-space degrees of freedom as a measure of change for other variables [1, 2]. Popular examples of internal times are a free massless scalar field or a variable that quantifies dust.

These variables are turned into operators when the theory is quantized and therefore appear in the state equations. They are of such a form that constraint equations can be rewritten as familiar evolution equations, for instance of Schrödinger or Klein–Gordon type. However, as part of the general problem of time [3, 4, 5] there is some arbitrariness involved in the choice of a particular internal time. Just as with coordinate time in classical general relativity or its cosmological models, one would therefore like to show that the choice of internal time does not affect predictions made from a quantum cosmological model. Only then can the model and its underlying theory be considered covariant.

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The question of covariance in internal-time formulations has rarely been studied, but some results are available [6, 7]. In this paper, we use semiclassical methods developed for effective constraints [8, 9, 10, 11, 12] in order to study this quation. We analyze an explicit model which permits two different choices of internal time. At a semiclassical level, the methods of effective constraints will be used to demonstrate covariance of moment corrections in the two internal-time formulations. However, the introduction of a propertime parameter turns out to be a more complicated step than usually appreciated. Such a parameter is important in order to relate evolution equations to observer frames, and it is often used in quantum cosmology in order to reformulate quantum evolution equations as effective or modified Friedmann equations.

In usual treatments of this question, it seems to be assumed implicitly that time reparameterization invariance is always guaranteed in homogeneous models of quantum cosmology because they are subject to just one constraint, the Hamiltonian constraint C with spatially constant lapse function. A single constraint always commutes with itself and therefore remains first class even if it is modified by quantum effects or fully quantized.

The last statement is correct, but it cannot always be applied to homogeneous quantum cosmology. In a Dirac quantization of a homogeneous cosmological model one replaces the classical constraint equation C = 0 by an equation $\hat{C}\psi = 0$ for physical states ψ . Since solving the state equation and constructing a suitable physical Hilbert space are complicated tasks, one often takes a shortcut and computes an "effective" equation which can more easily be analyzed, and which one expects to take the form of the classical Friedmann equation plus quantum corrections. There are different procedures for deriving such equations, but in some way they all make use of the expectation value $\langle \hat{C} \rangle$ of the constraint operator in a certain class of states. (The most systematic procedure of this type is the canonical effective one already mentioned; see for instance [13] for cosmological effective equations.)

The effective constraint equation $\langle \hat{C} \rangle = 0$ then resembles the Friedmann equation, as desired. But it does not imply that the state ψ used in it is a physical state satisfying $\hat{C}\psi =$ 0. The quantum constraint equation amounts to more than one independent expectationvalue equation, as systematically described in the formalism of effective constraints. For instance, if \hat{O} is some operator not equal to a number times the identity, the equation $\langle \hat{O}\hat{C} \rangle = 0$ is, generically, independent of the equation $\langle \hat{C} \rangle = 0$. The premise in the tacit assumption that time reparameterization invariance is always respected in homogeneous quantum cosmology because there is just a single constraint is therefore violated. Making sure that time reparameterization invariance, or more generally covariance, is still realized after quantization, or under which conditions it can be broken, is then an important task of quantum cosmology.

We will perform this task in the present paper for a specific model, and confirm that covariance cannot be taken for granted in deparameterized constructions. We then use the framework of effective constraints in order to compare different deparameterizations within the same setting, which is made possible by an analysis of the underlying gauge structure of quantum constraints. This discussion will lead us to a general definition of proper-time evolution in effective equations such that time reparameterization invariance is realized in moment corrections. Our new definition leads to proper-time evolution equations with moment corrections which are obtained from those in deparameterized evolution by a change of gauge. Compared with traditional derivations of proper-time evolution from deparameterized evolution, however, the covariant formulation predicts different quantum corrections for effective equations. A proper investigation of time reparameterization invariance is therefore crucial for a reliable determination of fluctuation corrections in quantum cosmological models.

In addition to moment corrections, different choices of internal or proper time may give rise to different factor ordering corrections. In contrast to moment corrections, these terms cannot be related by gauge transformations because effective constraints and the gauge they generate are computed for a fixed factor ordering. Factor ordering corrections therefore break covariance of internal-time formulations. In our specific model, all three time choices require different factor orderings of the constraint operator for real evolution generators. Time reparameterization invariance is therefore broken in internal-time quantum cosmology if all relevant corrections are taken into account, a result which makes the outcome of [6] more specific. However, the new proper-time evolution introduced here is time reparameterization invariant when compared with other choices of internal time. This evolution is unique in realizing the same type of covariance as in classical cosmological models, which is broken in internal-time evolution.

2 The model

Our cosmological model is isotropic, spatially flat, and has a cosmological constant Λ as well as a free, massless scalar field $\tilde{\phi}$. Its classical description is therefore given by the Friedmann equation

$$H^{2} = \frac{8\pi G}{3} \frac{\tilde{p}_{\tilde{\phi}}^{2}}{2a^{6}} + \Lambda$$
 (1)

for the scale factor a in $H = \dot{a}/a$ in terms of proper time.

We introduce the following canonical variables. (See [14] for a review of quantum cosmology and of the notation used here.) The Hubble parameter H is canonically conjugate to the "volume"

$$V := \frac{a^3}{4\pi G} \tag{2}$$

such that $\{H, V\} = 1$. The scalar field $\tilde{\phi}$ is canonically conjugate to the momentum $p_{\tilde{\phi}}$, such that $\{\tilde{\phi}, p_{\tilde{\phi}}\} = 1$. The cosmological constant Λ is canonically conjugate to a variable which we call T, such that $\{T, \Lambda\} = 1$.

The last statement may be unexpected. The cosmological constant is usually treated as just that, a constant that appears in Einstein's equation much like a fundamental constant such as G. However, it is mathematically consistent to treat it as the momentum of a variable T which does not appear in the action or Hamiltonian constraint of the theory. The momentum Λ of any such quantity is conserved in time, and therefore appears just as a constant in the field equations. We are not modifying the dynamics by introducing this new canonical pair (T, Λ) , nor are we trying to derive a mechanism for dark energy. We are merely using a mathematically equivalent formulation of the usual theory, as will be clear from the equations derived below. The new parameter T then presents to us a new option of a global internal time, which we can compare with the more standard global internal time $\tilde{\phi}$.

We note that we do not intend T to have physical meaning or to be measurable. This might be taken as a disadvantage of the formulation, but it is not that much different from the free scalar field $\tilde{\phi}$ for which no physical explanation is known. Both fields are introduced primarily for the purpose of serving as a global internal time. The variable T in fact has an advantage compared with $\tilde{\phi}$ because the energy density associated with it is just the cosmological constant, for which there is observational support. The energy density of a free scalar field, by contrast, has not been observed.

We have put tildes on the scalar symbols used so far. We now rescale these quantities so as to remove most numerical factors from our equations, just for the sake of convenience and in order not to distract from the important terms. We introduce

$$p_{\phi} := \frac{p_{\tilde{\phi}}}{\sqrt{12\pi G}} \tag{3}$$

and its canonical momentum ϕ . It is straightforward to confirm that the Friedmann equation (1) is equivalent to the constraint equation

$$C = -VH^2 + \frac{p_{\phi}^2}{V} + V\Lambda = 0 \tag{4}$$

in these new variables. We have multiplied the terms in the Friedmann equation with V in order to have energies rather than energy densities.

If we use this constraint to generate evolution equations with respect to proper time, we should remember the factor of $(4\pi G)^{-1}$ in the definition of V. The usual generator of proper-time evolution equations is

$$\tilde{C} = \frac{3}{8\pi G} \frac{a^3}{V} C = \frac{3}{2} C \,. \tag{5}$$

Our proper-time equations therefore differ by a factor of 3/2 from the usual ones, for instance

$$\frac{\mathrm{d}V}{\mathrm{d}\tau} = \{V, C\} = 2VH\tag{6}$$

which implies

$$H = \frac{1}{2V} \frac{\mathrm{d}V}{\mathrm{d}\tau} = \frac{3}{2a} \frac{\mathrm{d}a}{\mathrm{d}\tau} \tag{7}$$

with the promised factor of 3/2 compared with the usual $H = \dot{a}/a$. For completeness, we note the second classical evolution equation

$$\frac{\mathrm{d}H}{\mathrm{d}\tau} = -H^2 - \frac{p_{\phi}^2}{V^2} + \Lambda \approx -2(H^2 - \Lambda) \approx -2\frac{p_{\phi}^2}{V^2} \tag{8}$$

with the last two weak equalities indicating that the constraint (4) has been used.

3 Deparameterization

We deparameterize the model in two different ways, using the global internal times ϕ and T, respectively. We begin with the more familiar choice ϕ , solving C = 0 for the momentum

$$p_{\phi}(V, H, \Lambda) = -V\sqrt{H^2 - \Lambda}.$$
(9)

3.1 Scalar time

In this section, we quantize the model after deparameterization, so that there is an operator \hat{p}_{ϕ} acting on a (physical) Hilbert space of wave functions that do not depend on ϕ , for instance $\psi(V, T)$. All we assume about this operator for our semiclassical analysis is that it is Weyl ordered. The methods of [15, 16] then allow us to compute an effective Hamiltonian by formally expanding the expectation value

$$H_{\phi} := \langle p_{\phi}(\hat{V}, \hat{H}, \hat{\Lambda}) \rangle = \langle p_{\phi}(V + (\hat{V} - V), H + (\hat{H} - H), \Lambda + (\hat{\Lambda} - \Lambda)) \rangle$$
(10)

$$= p_{\phi}(V, H, \Lambda) + \sum_{a_1, a_2, a_3=2}^{\infty} \frac{1}{a_1! a_2! a_3!} \frac{\partial^{a_1 + a_2 + a_3} p_{\phi}(V, H, \Lambda)}{\partial V^{a_1} \partial H^{a_2} \partial \Lambda^{a_3}} \Delta(V^{a_1} H^{a_2} \Lambda^{a_3})$$
(11)

in $\hat{V} - V$, $\hat{H} - H$ and $\hat{\Lambda} - \Lambda$.

Although we use the same symbols V, H and Λ for our basic variables, they now refer to expectation values of the corresponding operators. In the expanded expression, in addition to expectation values, we have the moments

$$\Delta(O_1^{a_1}\cdots O_n^{a_n}) = \langle (\hat{O}_1 - O_1)^{a_1}\cdots (\hat{O}_n - O_n)^{a_n} \rangle_{\text{symm}}$$
(12)

(with totally symmetric or Weyl ordering) as independent variables. For instance, $\Delta(H^2) = (\Delta H)^2$ is the square of the *H*-fluctuation. If the cosmological constant is just a constant, the quantum state is an eigenstate of Λ , such that all moments including Λ vanish. However, we keep these moments in our equations for full generality. We will work exclusively with semiclassical approximations of the order \hbar , which includes corrections linear in second-order moments or terms with an explicit linear dependence on \hbar . We will ignore all higher-order moments as well as products of second-order moments. The elimination of higher-order terms will not always be indicated explicitly but holds throughout the paper. In our specific example, we have

$$H_{\phi} = -V\sqrt{H^{2} - \Lambda} - \frac{H}{\sqrt{H^{2} - \Lambda}}\Delta(VH) + \frac{1}{2}\frac{V\Lambda}{(H^{2} - \Lambda)^{3/2}}\Delta(H^{2})$$
(13)
+ $\frac{1}{2\sqrt{H^{2} - \Lambda}}\Delta(V\Lambda) - \frac{1}{2}\frac{VH}{(H^{2} - \Lambda)^{3/2}}\Delta(H\Lambda) + \frac{1}{8}\frac{V}{(H^{2} - \Lambda)^{3/2}}\Delta(\Lambda^{2}).$

The commutator of operators induces a Poisson bracket on expectation values and moments, seen as functions on the space of states. They can be derived from the definition

$$\{A,B\} = \frac{\langle [\hat{A},\hat{B}] \rangle}{i\hbar} \tag{14}$$

and the Leibniz rule. In particular, the classical bracket $\{H, V\} = 1$ still holds true for the expectation values, and expectation values have zero Poisson brackets with the moments. For Poisson brackets of two moments there are general equations [15, 17], but for small orders it is usually more convenient to compute brackets directly from (14). For instance,

$$\{\Delta(H^2), \Delta(V^2)\} = 4\Delta(VH), \qquad (15)$$

$$\{\Delta(H^2), \Delta(VH)\} = 2\Delta(H^2), \qquad (16)$$

$$\{\Delta(V^2), \Delta(VH)\} = -2\Delta(V^2).$$
(17)

These Poisson brackets give rise to the equations of motion

$$\frac{\mathrm{d}V}{\mathrm{d}\phi} = \{V, H_{\phi}\} = \frac{VH}{\sqrt{H^2 - \Lambda}} - \frac{\Lambda}{(H^2 - \Lambda)^{3/2}} \Delta(VH) + \frac{3}{2} \frac{VH\Lambda}{(H^2 - \Lambda)^{3/2}} \Delta(H^2) \qquad (18)$$
$$+ \frac{H}{2(H^2 - \Lambda)^{3/2}} \Delta(V\Lambda) - \frac{1}{2} \frac{V(2H^2 + \Lambda)}{(H^2 - \Lambda)^{5/2}} \Delta(H\Lambda) + \frac{3}{8} \frac{VH}{(H^2 - \Lambda)^{5/2}} \Delta(\Lambda^2)$$

and

$$\frac{\mathrm{d}H}{\mathrm{d}\phi} = -\sqrt{H^2 - \Lambda} + \frac{1}{2} \frac{\Lambda}{(H^2 - \Lambda)^{3/2}} \Delta(H^2) - \frac{1}{2} \frac{H}{(H^2 - \Lambda)^{3/2}} \Delta(H\Lambda) + \frac{1}{8} \frac{1}{(H^2 - \Lambda)^{3/2}} \Delta(\Lambda^2) ,$$
(19)

accompanied by equations of motion for the moments such as

$$\frac{\mathrm{d}\Delta(V^2)}{\mathrm{d}\phi} = 2\frac{H}{\sqrt{H^2 - \Lambda}}\Delta(V^2) - 2\frac{V\Lambda}{(H^2 - \Lambda)^{3/2}}\Delta(VH) + \frac{VH}{(H^2 - \Lambda)^{3/2}}\Delta(V\Lambda) \,. \tag{20}$$

Expectation values and moments are therefore dynamically coupled.

These equations can be compared with the classical Friedmann equation if we transform them to proper time. The usual way to do so is by using the chain rule after computing $d\phi/d\tau = \{\phi, C\}$. However, within the deparameterized setting, we do not have a quantumcorrected expression for C since we quantized p_{ϕ} after solving C = 0. The introduction of proper time in a deparameterized setting is therefore ambiguous. We will present two different alternatives in this section, none of which will turn out to be consistent by our general analysis in the next section.

The term in the constraint relevant for $\{\phi, C\}$ is p_{ϕ}^2/V , while the other two terms have zero Poisson brackets with ϕ . We tentatively introduce quantum corrections of this term by using the same methods that gave us the quantum corrected $p_{\phi}(V, H, \Lambda)$. The new term is then

$$C_{\phi} := \frac{p_{\phi}^2}{V} - 2\frac{p_{\phi}}{V^2}\Delta(Vp_{\phi}) + \frac{p_{\phi}^2}{V^3}\Delta(V^2) + \frac{1}{V}\Delta(p_{\phi}^2), \qquad (21)$$

leading to

$$\frac{d\phi}{d\tau} = \{\phi, -C_{\phi}\} = -2\frac{p_{\phi}}{V} + \frac{2}{V^2}\Delta(Vp_{\phi}) - \frac{2p_{\phi}}{V^3}\Delta(V^2)$$
(22)

$$= 2\sqrt{H^2 - \Lambda} + 2\frac{\sqrt{H^2 - \Lambda}}{V^2}\Delta(V^2) + \frac{2H}{V\sqrt{H^2 - \Lambda}}\Delta(VH) - \frac{\Lambda}{(H^2 - \Lambda)^{3/2}}\Delta(H^2) \quad (23)$$

$$-\frac{1}{V\sqrt{H^2-\Lambda}}\Delta(V\Lambda) + \frac{H}{(H^2-\Lambda)^{3/2}}\Delta(H\Lambda) - \frac{1}{4}\frac{1}{(H^2-\Lambda)^{3/2}}\Delta(\Lambda^2) + \frac{2}{V^2}\Delta(Vp_{\phi}).$$

(We use $-C_{\phi}$ in order to align forward motion of ϕ with forward motion of τ .) The chain rule then gives the proper-time equations

$$\frac{\mathrm{d}V}{\mathrm{d}\tau} = \frac{\mathrm{d}V}{\mathrm{d}\phi}\frac{\mathrm{d}\phi}{\mathrm{d}\tau} = 2VH + 2\Delta(VH) + 2\frac{VH\Lambda}{(H^2 - \Lambda)^2}\Delta(H^2)$$
(24)

$$-2\frac{Hp_{\phi}}{V^2\sqrt{H^2-\Lambda}}\Delta(V^2) + 2\frac{H}{V\sqrt{H^2-\Lambda}}\Delta(Vp_{\phi})$$
(25)

$$-\frac{V(H^2+\Lambda)}{(H^2-\Lambda)^2}\Delta(H\Lambda) + \frac{1}{2}\frac{VH}{(H^2-\Lambda)^2}\Delta(\Lambda^2)$$
(26)

and

$$\frac{\mathrm{d}H}{\mathrm{d}\tau} = -2(H^2 - \Lambda) - 2\frac{H}{V}\Delta(VH) + \frac{2\Lambda}{H^2 - \Lambda}\Delta(H^2)$$
(27)

$$+2\frac{p_{\phi}\sqrt{H^2-\Lambda}}{V^3}\Delta(V^2) - 2\frac{\sqrt{H^2-\Lambda}}{V^2}\Delta(Vp_{\phi})$$
(28)

$$+\frac{1}{V}\Delta(V\Lambda) - 2\frac{H}{H^2 - \Lambda}\Delta(H\Lambda) + \frac{1}{2}\frac{1}{H^2 - \Lambda}\Delta(\Lambda^2).$$
⁽²⁹⁾

Alternatively, we could square the deparameterized quantum Hamiltonian (13) and rearrange terms so as to make the expression look like the classical constraint plus moment terms. We obtain

$$0 = \frac{H_{\phi}^2}{V} - V^2(H^2 - \Lambda) - 2H\Delta(VH) + \frac{V\Lambda}{H^2 - \Lambda}\Delta(H^2)$$

$$+\Delta(V\Lambda) - \frac{VH}{H^2 - \Lambda}\Delta(H\Lambda) + \frac{1}{4}\frac{V}{H^2 - \Lambda}\Delta(\Lambda^2).$$
(30)

It is then possible to treat $H_{\phi} = \langle \hat{p}_{\phi} \rangle$ as the momentum of ϕ because, kinematically, $\{\phi, H_{\phi}\} = -i\hbar^{-1}\langle [\hat{\phi}, \hat{p}_{\phi}] \rangle = 1$ in the effective framework. This gives

$$\frac{\mathrm{d}\phi}{\mathrm{d}\tau} = -2\frac{H_{\phi}}{V} = 2\sqrt{H^2 - \Lambda} + \frac{2H}{V\sqrt{H^2 - \Lambda}}\Delta(VH) - \frac{\Lambda}{(H^2 - \Lambda)^{3/2}}\Delta(H^2)$$
(31)

$$-\frac{1}{V\sqrt{H^2-\Lambda}}\Delta(V\Lambda) + \frac{H}{(H^2-\Lambda)^{3/2}}\Delta(H\Lambda) - \frac{1}{4}\frac{1}{(H^2-\Lambda)^{3/2}}\Delta(\Lambda^2)$$
(32)

and

$$\frac{\mathrm{d}V}{\mathrm{d}\tau} = 2VH + 2\Delta(VH) + 2\frac{VH\Lambda}{(H^2 - \Lambda)^2}\Delta(H^2)$$
(33)

$$-\frac{V(H^2+\Lambda)}{(H^2-\Lambda)^2}\Delta(H\Lambda) + \frac{1}{2}\frac{VH}{(H^2-\Lambda)^2}\Delta(\Lambda^2), \qquad (34)$$

$$\frac{\mathrm{d}H}{\mathrm{d}\tau} = -2(H^2 - \Lambda) - 2\frac{H}{V}\Delta(VH) + \frac{2\Lambda}{H^2 - \Lambda}\Delta(H^2)$$
(35)

$$+\frac{1}{V}\Delta(V\Lambda) - 2\frac{H}{H^2 - \Lambda}\Delta(H\Lambda) + \frac{1}{2}\frac{1}{H^2 - \Lambda}\Delta(\Lambda^2).$$
(36)

These equations are different than what we obtained with the first choice of C.

3.2 Cosmological time

For internal time T, we solve the constraint C = 0 for the momentum

$$\Lambda(V, H, p_{\phi}) = H^2 - \frac{p_{\phi}^2}{V^2}.$$
(37)

Its semiclassical quantization gives the Hamiltonian

$$H_T = H^2 - \frac{p_{\phi}^2}{V^2} + \Delta(H^2) - \frac{3p_{\phi}^2}{V^4}\Delta(V^2) - \frac{1}{V^2}\Delta(p_{\phi}^2) + 4\frac{p_{\phi}}{V^3}\Delta(Vp_{\phi}), \qquad (38)$$

generating equations of motion

$$\frac{\mathrm{d}V}{\mathrm{d}T} = -2H\tag{39}$$

and

$$\frac{\mathrm{d}H}{\mathrm{d}T} = 2\frac{p_{\phi}^2}{V^3} + 12\frac{p_{\phi}^2}{V^5}\Delta(V^2) + \frac{2}{V^3}\Delta(p_{\phi}^2) - 12\frac{p_{\phi}}{V^4}\Delta(Vp_{\phi}).$$
(40)

We attempt to transform to proper time using

$$\frac{\mathrm{d}T}{\mathrm{d}\tau} = \{T, -C\} = -V.$$
(41)

No quantum corrections appear in this equation because the constraint is linear in Λ . We obtain

$$\frac{\mathrm{d}V}{\mathrm{d}\tau} = 2VH\tag{42}$$

and

$$\frac{\mathrm{d}H}{\mathrm{d}\tau} = -2\frac{p_{\phi}^2}{V^2} - 12\frac{p_{\phi}^2}{V^4}\Delta(V^2) - \frac{2}{V^2}\Delta(p_{\phi}^2) + 12\frac{p_{\phi}}{V^3}\Delta(Vp_{\phi})$$
(43)

$$\approx -2(H^2 - \Lambda) - 2\Delta(H^2) - 6\frac{H^2 - \Lambda}{V^2}\Delta(V^2) + 4\frac{p_{\phi}}{V^3}\Delta(Vp_{\phi}).$$
(44)

In the last step, we have used the constraint $H_T - \Lambda = 0$ in order to bring the equation closer to the form seen with ϕ as internal time. Nevertheless, there is no obvious relationship between the two deparameterizations (in either one of the two versions presented for the scalar time), and covariance remains unclear.

3.3 A new scalar time

A formal difference between the scalar and cosmological choices of internal times is the linear appearance of the time momentum in the former case, compared with the quadratic appearence in the latter. In order to show that this is not the reason for the disagreement of proper-time evolutions, we modify the treatment of scalar time by applying a canonical transformation: We replace ϕ and p_{ϕ} by $q := \frac{1}{2}\phi/p_{\phi}$ and $p := p_{\phi}^2$. The constraint

$$C = -VH^2 + \frac{p}{V} + V\lambda = 0 \tag{45}$$

is then linear in p which we now use as the momentum of internal time q.

Proceeding as before, we have the quantum Hamiltonian

$$H_q = V^2 (H^2 - \Lambda) + (H^2 - \Lambda)\Delta(V^2) + 4VH\Delta(VH) + V^2\Delta(H^2) - 2V\Delta(V\Lambda)$$
(46)

and the internal-time evolution equations

....

$$\frac{\mathrm{d}V}{\mathrm{d}q} = -2V^2H - 2H\Delta(V^2) - 4V\Delta(VH), \qquad (47)$$

$$\frac{\mathrm{d}H}{\mathrm{d}q} = 2V(H^2 - \Lambda) + 4H\Delta(VH) + 2V\Delta(H^2) - 2\Delta(V\Lambda).$$
(48)

Internal time q is tentatively related to proper time τ by

$$\frac{\mathrm{d}q}{\mathrm{d}\tau} = -\frac{1}{V}\,,\tag{49}$$

and we obtain proper-time equations

$$\frac{\mathrm{d}V}{\mathrm{d}\tau} = 2VH + 2\frac{H}{V}\Delta(V^2) + 4\Delta(VH), \qquad (50)$$

$$\frac{\mathrm{d}H}{\mathrm{d}\tau} = -2(H^2 - \Lambda) - 4\frac{H}{V}\Delta(VH) - 2\Delta(H^2) + \frac{2}{V}\Delta(V\Lambda)$$
(51)

which agree with none of the previous versions.

4 Gauge structure

Covariance is a property of the gauge nature of a theory. For systems with a single Hamiltonian constraint C, as in our classical model, reparameterization invariance is guaranteed by the fact that we always have $\{C, C\} = 0$ and the constraint is first class. It generates a gauge transformation which corresponds to reparameterization invariance of the time variable, be it proper time as the gauge parameter in $d/d\tau = \{\cdot, C\}$ or internal time. Even if the classical constraint is modified by putative quantum corrections, as a single constraint it always commutes with itself and reparameterization invariance should be respected. Our examples contradict this expectation.

The discrepancy is resolved if we remember that quantization introduces new degrees of freedom, parameterized in the effective formulation by fluctuations, covariances and higher moments of a state. If fluctuations are included as in our examples, the system is therefore equipped with a different, enlarged phase space.

For the same reduction of degrees of freedom to result in this enlarged setting as in the classical theory, there must also be additional constraints. If a canonical pair such as (ϕ, p_{ϕ}) is eliminated by solving the classical constraint and factoring out its gauge flow, not only the expectation values of ϕ and p_{ϕ} must be eliminated by quantized constraints but also the moments involving ϕ or p_{ϕ} . On the quantum phase space, these latter variables are independent of the expectation values, and therefore require new constraints in order to be eliminated.

4.1 Effective constraints

Using the canonical effective description, additional constraints appear automatically for any first-class classical constraint C. If \hat{C} is an operator with classical limit C, about which we again assume only that it is Weyl ordered, not only the expectation value

$$C_1 := \langle \hat{C} \rangle = 0 \tag{52}$$

is a constraint, but also all expressions of the form

$$C_f := \langle (\hat{f} - f)\hat{C} \rangle = 0 \tag{53}$$

where f is an arbitrary classical phase-space function and \hat{f} its (Weyl-ordered) quantization. For $f \neq 1$, the equation $C_f = 0$ is independent of $C_1 = 0$ on the quantum phase space. There are therefore infinitely many new constraints C_f , which can conveniently be organized by using for f polynomials in some set of basic phase-space variables.

Just as expectation values of Hamiltonians used in the deparameterized models, the effective constraints can be expanded in moments. We have

$$C_1(O_1, \dots, O_n, \Delta(\cdot)) = C(O_1, \dots, O_n)$$

$$+ \sum_{a_1, \dots, a_n} \frac{1}{a_1! \cdots a_n!} \frac{\partial^{a_1 + \dots + a_n} C(O_1, \dots, O_n)}{\partial O_1^{a_1} \cdots \partial O_n^{a_n}} \Delta(O^{a_1} \cdots O^{a_n})$$
(54)

where the basic variables are called $O_1, \ldots, O_n, \Delta(\cdot)$ denotes their moments, and C is the classical constraint. Similarly, any C_f can be expanded in this way, but it usually requires reordering terms because $\hat{f}\hat{C}$ is not necessarily Weyl ordered for Weyl ordered \hat{f} and \hat{C} . We will see this more explicitly in our examples.

4.2 Cosmological model

We now compute effective constraints up to second-order moments for our constraint (4). This order requires us to accompany $C_1 = \langle \hat{C} \rangle$ by all constraints C_f with f linear in basic variables. We obtain seven constraints

$$C_{1} = -VH^{2} + \frac{p_{\phi}^{2}}{V} + V\Lambda + \frac{p_{\phi}^{2}}{V^{3}}\Delta(V^{2}) - 2H\Delta(VH) - V\Delta(H^{2})$$

$$+ \frac{1}{V}\Delta(p_{\phi}^{2}) - 2\frac{p_{\phi}}{V^{2}}\Delta(Vp_{\phi}) + \Delta(V\Lambda),$$
(55)

$$C_{V} = -\left(H^{2} + \frac{p_{\phi}^{2}}{V^{2}} - \Lambda\right) \Delta(V^{2}) - 2VH\left(\Delta(VH) - \frac{1}{2}i\hbar\right)$$

$$+2\frac{p_{\phi}}{V}\Delta(Vp_{\phi}) + V\Delta(V\Lambda),$$
(56)

$$C_H = -2VH\Delta(H^2) - \left(H^2 + \frac{p_{\phi}^2}{V^2} - \Lambda\right) \left(\Delta(VH) + \frac{1}{2}i\hbar\right)$$
(57)

$$+2\frac{p_{\phi}}{V}\Delta(Hp_{\phi}) + V\Delta(H\Lambda),$$

$$C_{\phi} = -\left(H^{2} + \frac{p_{\phi}^{2}}{V^{2}} - \Lambda\right)\Delta(V\phi) - 2VH\Delta(H\phi)$$

$$+2\frac{p_{\phi}}{V}\left(\Delta(\phi p_{\phi}) + \frac{1}{2}i\hbar\right) + V\Delta(\phi\Lambda),$$
(58)

$$C_{p_{\phi}} = -\left(H^2 + \frac{p_{\phi}^2}{V^2} - \Lambda\right) \Delta(Vp_{\phi}) - 2VH\Delta(Hp_{\phi}) + 2\frac{p_{\phi}}{V}\Delta(p_{\phi})^2 + V\Delta(p_{\phi}\Lambda), \quad (59)$$

$$C_T = -\left(H^2 + \frac{p_{\phi}^2}{V^2} - \Lambda\right) \Delta(VT) - 2VH\Delta(HT) + 2\frac{p_{\phi}}{V}\Delta(p_{\phi}T)$$
(60)

$$+V\left(\Delta(\Lambda T) + \frac{1}{2}i\hbar\right),$$

$$C_{\Lambda} = -\left(H^{2} + \frac{p_{\phi}^{2}}{V^{2}} - \Lambda\right)\Delta(V\Lambda) - 2VH\Delta(H\lambda) + 2\frac{p_{\phi}}{V}\Delta(p_{\phi}\Lambda) + V\Delta(\Lambda^{2}). \quad (61)$$

The terms of $\frac{1}{2}i\hbar$ are from reordering to Weyl ordered moments. Some of the effective constraints are therefore complex, and so will be some of the moments after solving the constraints. This property is not problematic because we have not eliminated any variables yet and are therefore still in the kinematical setting. As shown in [8, 9], after solving the constraints and factoring out their gauge flows one can impose reality conditions on the resulting physical moments. Real-valued observables are then obtained, corresponding to expressions taken in the physical Hilbert space.

Also in [8, 9], it has been shown that the effective constraints form a first-class system. Therefore, they generate gauge transformations. However, the phase space of expectation values and moments up to a certain order is not always symplectic, and the number of constraints is not always equal to the number of independent gauge transformations. (See [18] for a discussion of first-class constraints in non-symplectic systems.) In particular, a smaller number of gauge-fixing conditions may be required if one would like to fix the gauge of a given set of constraints on a Poisson manifold.

4.3 Effective deparameterization

Deparameterization with respect to a given internal time such as ϕ amounts to a specific choice of gauge fixing. After deparameterization, ϕ , just as the usual t in non-relativistic quantum mechanics, is no longer represented by an operator but only appears as a parameter in the theory. It is not subject to quantum fluctuations and does not have quantum correlations with other variables. These properties are reflected in the gauge-fixing conditions

$$\Delta(\phi^2) = \Delta(V\phi) = \Delta(H\phi) = \Delta(\phi T) = \Delta(\phi \Lambda) = 0$$
(62)

which, as shown in [10, 11], suffice to fix the effective constraints C_f with linear f.

The remaining covariance of ϕ with p_{ϕ} is not zero but takes the complex value

$$\Delta(\phi p_{\phi}) = -\frac{1}{2}i\hbar \tag{63}$$

as a consequence of $C_{\phi} = 0$ together with the gauge-fixing conditions. This complex value plays only a formal role, but it is useful because it means that the uncertainty relation

$$\Delta(\phi^2)\Delta(p_{\phi})^2 - \Delta(\phi p_{\phi})^2 \ge \frac{\hbar^2}{4}$$
(64)

is still respected even with $\Delta(\phi^2) = 0$.

4.3.1 Scalar time

We proceed to solving the remaining effective constraints. From $C_V = 0$, we obtain

$$\Delta(Vp_{\phi}) = \frac{1}{2} \frac{V}{p_{\phi}} \left(\left(H^2 + \frac{p_{\phi}^2}{V^2} - \Lambda \right) \Delta(V^2) + 2VH \left(\Delta(VH) - \frac{1}{2}i\hbar \right) - V\Delta(V\Lambda) \right); \quad (65)$$

from $C_H = 0$,

$$\Delta(Hp_{\phi}) = \frac{1}{2} \frac{p_{\phi}}{V} \left(2VH\Delta(H^2) + \left(H^2 + \frac{p_{\phi}^2}{V^2} - \Lambda\right) \left(\Delta(VH) + \frac{1}{2}i\hbar\right) - V\Delta(H\Lambda) \right); \quad (66)$$

from $C_{\Lambda} = 0$,

$$\Delta(p_{\phi}\Lambda) = \frac{1}{2} \frac{p_{\phi}}{V} \left(\left(H^2 + \frac{p_{\phi}^2}{V^2} - \Lambda \right) \Delta(V\Lambda) + 2VH\Delta(H\Lambda) - V\Delta(\Lambda^2) \right);$$
(67)

and from $C_{p_{\phi}} = 0$,

$$\Delta(p_{\phi}^2) = \frac{1}{2} \frac{p_{\phi}}{V} \left(\left(H^2 + \frac{p_{\phi}^2}{V^2} - \Lambda \right) \Delta(Vp_{\phi}) + 2VH\Delta(Hp_{\phi}) - V\Delta(p_{\phi}\Lambda) \right)$$
(68)

$$= \frac{1}{4} \frac{V^2}{p_{\phi}^2} \left(H^2 + \frac{p_{\phi}^2}{V^2} - \Lambda \right) \Delta(V^2) + \frac{V^4 H^2}{p_{\phi}^2} \Delta(H^2) + \frac{V^3 H}{p_{\phi}^2} \left(H^2 + \frac{p_{\phi}^2}{V^2} - \Lambda \right) \Delta(VH)$$

$$-\frac{V^3}{p_{\phi}^2}\left(H^2 + \frac{p_{\phi}^2}{V^2} - \Lambda\right)\Delta(V\Lambda) - \frac{V^4H}{p_{\phi}^2}\Delta(H\Lambda) + \frac{1}{4}\frac{V^4}{p_{\phi}^2}\Delta(\Lambda^2).$$
(69)

Notice again that the moments $\Delta(Vp_{\phi})$ and $\Delta(Hp_{\phi})$ are complex. The reason is that we are in the process of deparameterizing by ϕ , which eliminates all moments related to the canonical pair (ϕ, p_{ϕ}) , including their covariances with other variables. In the complex moments, p_{ϕ} is therefore not an independent variable anymore. It is a function of V, H, Λ and the moments owing to the constraint $C_1 = 0$. While $\hat{V}\hat{p}_{\phi}$ is a Hermitian operator when V and p_{ϕ} are independent, it is no longer Hermitian in this ordering if p_{ϕ} is a function of H after solving $C_1 = 0$. The complex contributions to $\Delta(Vp_{\phi})$ and $\Delta(Hp_{\phi})$ implicitly describe the ordering obtained after solving the constraints. Note that $\Delta(p_{\phi}\Lambda)$ remains real, which is consistent with the fact that p_{ϕ} does not depend on T after $C_1 = 0$ is solved. (See also [19] for a related discussion of complex moments.)

All p_{ϕ} -moments can now be eliminated from the remaining constraint $C_1 = 0$, as appropriate for a system deparameterized with respect to ϕ . The resulting expression can be compared with the evolution generator on the physical Hilbert space, where no operators for ϕ and p_{ϕ} exist. However, there is one last step before such a comparison can be done. We have introduced gauge-fixing conditions, and must therefore make sure that the evolution generator preserves these conditions. Usually, such a generator is not the remaining (unfixed) constraint C_1 but a linear combination of all the constraints of the system. (The gauge fixing requires us to use a specific lapse function N on the quantum phase space.)

Using the methods of [11, 20], one can check that, in the present example, the unique generator respecting the gauge-fixing conditions is of the form

$$NC = \frac{1}{2p_{\phi}} \left((VC)_{1} - \frac{1}{2p_{\phi}} (VC)_{p_{\phi}} - \frac{1}{2p_{\phi}} \frac{\partial p_{\phi}}{\partial V} (VC)_{V} - \frac{1}{2p_{\phi}} \frac{\partial p_{\phi}}{\partial H} (VC)_{H} \right)$$

$$- \frac{1}{2p_{\phi}} \frac{\partial p_{\phi}}{\partial \Lambda} (VC)_{\Lambda} - \frac{1}{2p_{\phi}} \frac{\partial p_{\phi}}{\partial T} (VC)_{T} \right)$$

$$(70)$$

where $(VC)_f$ are defined just like the previous effective constraints but with $\hat{V}\hat{C}$ inserted instead of \hat{C} . The factor of \hat{V} removes the 1/V in the quadratic kinetic term p_{ϕ}^2/V in C. We emphasize that we are still dealing with the original system of effective constraints because any $(VC)_f$ can be written as a linear combination of the C_f to the same order. For instance,

$$(VC)_1 = \langle (V + (\hat{V} - V))\hat{C} \rangle = VC_1 + C_V$$
 (71)

and

$$(VC)_V = \langle (\hat{V} - V)(V + (\hat{V} - V))\hat{C} \rangle = VC_V + \Delta(V^2)C_1.$$
 (72)

For our present purposes, it suffices to justify the combination (70) of constraints by confirming that the resulting generator

$$NC = \frac{p_{\phi} - V\sqrt{H^2 - \Lambda}}{2p_{\phi}} \left(p_{\phi} + V\sqrt{H^2 - \Lambda} \right) + \frac{H}{\sqrt{H^2 - \Lambda}} \Delta(VH) - \frac{1}{2} \frac{V\Lambda}{(H^2 - \Lambda)^{3/2}} \Delta(H^2) - \frac{1}{2\sqrt{H^2 - \Lambda}} \Delta(V\Lambda) + \frac{1}{2} \frac{VH}{(H^2 - \Lambda)^{3/2}} \Delta(H\Lambda) - \frac{1}{8} \frac{V}{(H^2 - \Lambda)^{3/2}} \Delta(\Lambda^2)$$
(73)

indeed preserves the gauge-fixing conditions: all p_{ϕ} -moments have cancelled out. Moreover, solving NC = 0 for p_{ϕ} gives an expression identical with the deparameterized ϕ -Hamiltonian (13). We therefore confirm that deparemeterization can be performed before or after quantization, with equivalent results.

4.3.2 Cosmological time

Deparameterization of the effective constraints with respect to T is done by using the gauge-fixing conditions

$$\Delta(T^2) = \Delta(VT) = \Delta(HT) = \Delta(\phi T) = \Delta(p_{\phi}T) = 0$$
(74)

which implies $\Delta(T\Lambda) = -\frac{1}{2}i\hbar$ using $C_T = 0$. As before, we can solve all constraints for the Λ -moments, but we do not need the explicit expressions because the relevant generator,

$$\left(V^{-1}C'\right)_{1} = -H^{2} + \frac{p_{\phi}^{2}}{V^{2}} + \Lambda - \Delta(H^{2}) + 3\frac{p_{\phi}^{2}}{V^{4}}\Delta(V^{2}) - 4\frac{p_{\phi}}{V^{3}}\Delta(Vp_{\phi}) + \frac{1}{V^{2}}\Delta(p_{\phi}^{2})$$
(75)

contains no such moments. Solving $(V^{-1}C')_1 = 0$ for $\Lambda = H_T$ gives an expression for the *T*-Hamiltonian identical with (38).

Similarly to the scalar case, the momentum Λ appears with a factor of V, which leads to the modified effective constraint $(V^{-1}C')_1$. We have indicated by the prime on C' a change of factor ordering with respect to the original Weyl-ordered constraint operator \hat{C} . In order for $(V^{-1}C')_1$ to be real, we need a symmetric ordering of the contribution $\hat{V}^{-1}(\hat{V}\hat{H}^2)'$ with some ordering of $\hat{V}\hat{H}^2$ again indicated by the prime. The product with \hat{V}^{-1} is not symmetric if Weyl-ordering is used for $(\hat{V}\hat{H}^2)'$, but it is symmetric if we instead use

$$\hat{V}\hat{H}^2 = \frac{1}{3}(\hat{V}\hat{H}^2 + \hat{H}\hat{V}\hat{H} + \hat{H}^2\hat{V}) - i\hbar\hat{H} = (\hat{V}\hat{H}^2)_{\text{Weyl}} - i\hbar\hat{H}.$$
(76)

Indeed, with the subtraction of $i\hbar\hat{H}$ in the reordered constraint $\hat{C}' = \hat{C} - i\hbar\hat{H}$, we have

$$\left(V^{-1}C'\right)_{1} = \langle (V^{-1} - V^{-2}(\hat{V} - V))(\hat{C} - i\hbar\hat{H})\rangle = \frac{C_{1}}{V} - \frac{C_{V} - i\hbar VH}{V^{2}}$$
(77)

as a real expression of the effective constraints, where C_V has imaginary part $\hbar V H$.

Unlike the generator of deparameterized evolution in the scalar model, the generator for cosmological time is *not* a linear combination of the original effective constraints because $i\hbar H/V$ is not of such a form. The two deparameterized models are therefore realized within the same effective constrained system only if we ignore reordering contributions with an explicit dependence on \hbar . The moment corrections in the two models are related by a gauge transformation and therefore provide the same effects in observables. However, \hbar -dependent terms are not related by gauge transformations and lead to different effects in observables. For semiclassical states, for which our analysis is valid, second-order moments are generically of the order \hbar , and it is not possible to ignore factor ordering corrections compared with moment corrections. The two different internal times therefore lead to different predictions, and time reparameterization invariance is broken.

4.4 Proper time

Using effective constraints, we have rederived the deparameterized Hamiltonians (13) and (38) for our model with two different choices of internal time. The agreement with derivations in deparameterized models in the preceding Sec. 3 demonstrates that it does not

matter whether we deparameterize the classical theory and then quantize the internal-time Hamiltonians, or whether we quantize first using effective constraints and then deparameterize. At least at the semiclassical level used here, deparameterization therefore commutes with quantization.

Moreover, we have realized the two internal-time models as two different gauge fixings of the same constrained system, up to reordering terms. Since the constraints are first class, the observable content of the models does not depend on the particular gauge fixing used to derive it, as long as only moment corrections are considered. (Explicit gauge transformations of moments relating the models can be derived as in [11].) We have therefore demonstrated in our quantized cosmological model how covariance can in principle be realized, in the sense that the two internal-time versions derived in Sec. 3 would be equivalent to each other. However, in our explicit example, covariance is broken by factor ordering corrections, which appear whenever the momenta of two internal times appear in the constraint with different phase-space dependent factors. However, this result, which we consider to be rather important, cannot explain the mismatch of proper-time evolutions we found in Sec. 3 because this mismatch appears even for moment corrections. The existence of gauge transformations that successfully transform the moment corrections in deparameterized effective constraints, at first sight, makes the disagreement of their proper-time evolutions only more puzzling.

However, supplied with the methods of effective constraints, we can now revisit this question with a complete view on the gauge structure. Our first attempt to derive propertime evolution from internal-time evolution required an expression for $d\phi/d\tau$ or $dT/d\tau$. Since there is no τ in the deparameterized theory, such an expression can only come from the original constraint. It may be amended by different versions of moment corrections, as seen in the scalar example, but it is always closely related to the original gauge generator which we have now called C_1 .

At this point, we can see the reason for our problem of mismatched proper-time evolutions. A deparameterized model is equivalent to a specific gauge fixing of effective constraints. The gauge fixing must be preserved by evolution in the model, which requires a specific combination of effective constraints as evolution generator. If the classical constraint is not linear in the momentum of internal time, or if there are phase-space dependent factors such as V or 1/V of the momentum of internal time, the evolution generator preserving the gauge fixing is not equal to the effective constraint C_1 used for proper time. The only generator consistent with the gauge-fixing conditions is the deparameterized Hamiltonian (or this Hamiltonian multiplied with a quantum phase-space function not depending on internal time and its momentum).

In this way, only the deparameterized evolution can be described within a deparameterized model. It is impossible to transform this evolution to proper time and still have reparameterization invariance or covariance. Referring to the chain rule in order to transform from an internal time to proper time is meaningless in this context of multiple constraints. The 1-parameter chain rule $d/d\tau = (d\phi/d\tau)d/d\phi$ is valid only if evolution is described by a unique 1-dimensional trajectory. This is the case in the classical theory, in which there is just one constraint, but not in the quantum theory in which expectation values and moments provide independent constraints. In order to apply the 1-parameter chain rule, one would first have to select a unique trajectory generated by a distinguished linear combination of the constraints. But once a specific linear combination has been selected, it corresponds to a fixed choice of time. Transformations between different time choices are then no longer possible.

There is a way to obtain proper-time evolution from the effective constraints. Proper time is not a phase-space variable, and therefore it does not correspond to a natural gauge fixing of the effective constraints. Instead of fixing the gauge of linear constraints C_f , we compute invariant expectation values and moments, or Dirac observables of this subset of constraints. Up to terms of higher order in \hbar including products of second-order moments, as always in this paper, we have the invariants

$$\mathcal{V} = V - \frac{VH}{p_{\phi}} \Delta(V\phi) - \frac{V^2}{p_{\phi}} \Delta(H\phi) + \frac{V^3 \Lambda}{2p_{\phi}^2} \Delta(\phi^2), \qquad (78)$$

$$\mathcal{H} = H + 2\frac{VH}{p_{\phi}}\Delta(H\phi) - \frac{V}{p_{\phi}}\Delta(\phi\Lambda) + H\Delta(\phi^2)$$
(79)

as well as

$$\Delta(\mathcal{V}^2) = \Delta(V^2) - 2\frac{V^2 H}{p_{\phi}}\Delta(V\phi) + \frac{V^4 H^2}{p_{\phi}^2}\Delta(\phi^2), \qquad (80)$$

$$\Delta(\mathcal{VH}) = \Delta(VH) + \frac{p_{\phi}}{V}\Delta(V\phi) - \frac{V^2H}{p_{\phi}}\Delta(H\phi) - HV\Delta(\phi^2), \qquad (81)$$

$$\Delta(\mathcal{H}^2) = \Delta(H^2) + 2\frac{p_{\phi}}{V}\Delta(H\phi) + \frac{p_{\phi}^2}{V^2}\Delta(\phi^2), \qquad (82)$$

$$\Delta(\mathcal{V}p_{\phi}) = \Delta(Vp_{\phi}) - \frac{V^2 H}{p_{\phi}} \Delta(\phi p_{\phi}).$$
(83)

Moreover, p_{ϕ} , Λ , $\Delta(p_{\phi}^2)$, $\Delta(p_{\phi}\Lambda)$ and $\Delta(\Lambda^2)$ are invariant. Note that $\Delta(\mathcal{V}p_{\phi})$ in (83) is real even if ϕ is used as internal time because the non-zero imaginary parts of $\Delta(Vp_{\phi})$ and $\Delta(\phi p_{\phi})$, according to (65) and (63) cancel out completely.

These combinations of expectation values and moments are invariant to second-order moments under gauge transformations generated by effective constraints C_f with f linear in basic variables. In the gauge (62) of a formulation deparameterized by internal time ϕ , they are equal to the kinematical expectation values and moments of the same type and thus provide an invariant extension of these variables. In the gauge of some other internal time such as T, with conditions (74), there are additional non-zero moments compared with the simple kinematical expressions V, H, $\Delta(V^2)$, $\Delta(VH)$, $\Delta(H^2)$ and $\Delta(Vp_{\phi})$. If one analyzes a model using different internal times, such as ϕ and T in the present case, one should therefore not directly compare moments of the same type, but combinations as dictated by invariant moments. For instance, the fluctuation $\Delta(V^2)$ computed with internal time ϕ represents the same observable (with respect to linear constraints C_f) as $\Delta(V^2) - 2(V^2H/p_{\phi})\Delta(V\phi) + (V^4H^2/p_{\phi}^2)\Delta(\phi^2)$ computed with internal time T. The remaining constraint C_1 written in terms of invariant expectation values and moments is

$$\mathcal{C} = -\mathcal{V}\mathcal{H}^2 + \frac{p_{\phi}^2}{\mathcal{V}^2} + \mathcal{V}\Lambda - \mathcal{V}\Delta(\mathcal{H}^2) - 2\mathcal{H}\Delta(\mathcal{V}\mathcal{H}) + \frac{p_{\phi}^2}{\mathcal{V}^3}\Delta(\mathcal{V}^2) + \frac{1}{\mathcal{V}}\Delta(p_{\phi}^2) - 2\frac{p_{\phi}}{\mathcal{V}^2}\Delta(\mathcal{V}p_{\phi}) + \Delta(\mathcal{V}\Lambda) + i\hbar H + \frac{p_{\phi}^2}{\mathcal{V}^3}\Delta(\mathcal{V}^2) + \frac{1}{\mathcal{V}}\Delta(p_{\phi}^2) - 2\frac{p_{\phi}}{\mathcal{V}^2}\Delta(\mathcal{V}p_{\phi}) + \frac{1}{\mathcal{V}}\Delta(\mathcal{V}\Lambda) + i\hbar H + \frac{1}{\mathcal{V}}\Delta(\mathcal{V}\Lambda) +$$

The moment corrections are of the same form that C_1 has in terms of the kinematical expectation values and moments. However, the transformation to invariant moments leads to an imaginary part $\hbar H$ which indicates that the Weyl-ordered operator used for C_1 was not of the correct ordering. Similarly to (76), we have

$$\hat{H}^{2}\hat{V} = \frac{1}{3}(\hat{V}\hat{H}^{2} + \hat{H}\hat{V}\hat{H} + \hat{H}^{2}\hat{V}) + i\hbar\hat{H} = (\hat{V}\hat{H}^{2})_{\text{Weyl}} + i\hbar\hat{H}.$$
(85)

If we use the ordering $(\hat{V}\hat{H}^2)'' = \hat{H}^2\hat{V}$ in a reordered constraint operator \hat{C}'' , we have $\hat{C}'' = \hat{C}_{Weyl} - i\hbar\hat{H}$ and the imaginary parts in $\langle \hat{C}'' \rangle$ cancel out after transformation to invariant expectation values and moments:

$$\mathcal{C}'' = -\mathcal{V}\mathcal{H}^2 + \frac{p_{\phi}^2}{\mathcal{V}^2} + \mathcal{V}\Lambda - \mathcal{V}\Delta(\mathcal{H}^2) - 2\mathcal{H}\Delta(\mathcal{V}\mathcal{H}) + \frac{p_{\phi}^2}{\mathcal{V}^3}\Delta(\mathcal{V}^2) + \frac{1}{\mathcal{V}}\Delta(p_{\phi}^2) - 2\frac{p_{\phi}}{\mathcal{V}^2}\Delta(\mathcal{V}p_{\phi}) + \Delta(\mathcal{V}\Lambda) .$$
(86)

We have not found an independent argument why the ordering of \hat{C}'' should be used for proper-time evolution. The appearance of this particular ordering is therefore rather surprising, as is the fact that it is different from the two orderings required for scalar and cosmological internal times.

With a real-valued effective constraint C'' in terms of invariants, we can finally introduce proper-time evolution. We do not introduce gauge-fixing conditions but explicitly select the lapse function of the generic evolution generator

$$NC_{\text{eff}} = N_1 C_1'' + \sum_f N_f C_f'' = \langle (N_1 + N_f (\hat{f} - f)) \hat{C}'' \rangle = \langle \hat{N} \hat{C}'' \rangle$$
(87)

by setting all $N_f = 0$ for $f \neq 1$ and $N_1 = 1$. This choice implements the feature that proper time, in a geometrical formulation, corresponds to a lapse function N = 1. At the operator level, we should then have $\hat{N} = 1$ without any contributions from $\hat{f} - f$. Proper-time evolution equations are then generated by \mathcal{C}'' , which is $\langle \hat{C}'' \rangle$ expressed in invariant expectation values and moments. Just as in classical equations, it is not necessary to compute complete Dirac observables which are also invariant under the flow generated by \mathcal{C}'' , since we can directly interpret proper-time trajectories in geometrical terms. The tedious constructions of physical Hilbert spaces in standard treatments of canonical quantum cosmology are, at the effective level, replaced by invariance conditions with respect to the flow generated by C_f , combined with reality conditions on \mathcal{C}'' .

Proper time can therefore be implemented within the effective constrained system, but it amounts to a gauge fixing different from most deparameterized models. If we consider only moment corrections, there are gauge transformations between proper-time and all deparameterized models within the effective constrained system and reparameterization invariance is preserved, including proper time. Factor-ordering corrections generically break covariance. However, no gauge transformation to proper time exists within a deparameterized model, in which the gauge fixing can no longer be changed. This is the case even if factor ordering terms are ignored, so that covariance is more strongly broken in such cases.

Other coordinate times, such as conformal time, can be implemented in the same way by still using $N_f = 0$ but $N \neq 1$ a function of expectation values. Their evolution generators are given by $\mathcal{NC''}$ where \mathcal{N} is obtained by replacing expectation values in N by their invariant analogs. No new factor ordering of \hat{C} is required because we just multiply the proper-time generator $\mathcal{C''}$ with a function of invariants, which keeps the expression real. Our definition of proper-time therefore allows the same changes of time coordinates as in the classical theory and is, in this sense, time reparameterization invariant. This invariance is broken only if we try to compare coordinate time with internal time.

5 Discussion

We have pointed out that time reparameterization invariance of effective equations is not guaranteed after quantization even in systems with a single constraint, and illustrated this often overlooked property in a specific cosmological model. Our detailed analysis of the underlying quantum gauge system has led us to a new procedure in which one can implement proper-time evolution at the effective level. This new definition includes all analogs of different classical choices of coordinate time and is time reparameterization invariant in this sense. Moreover, our procedure unifies models with coordinate times and internal times because they are all obtained from the same first-class constrained system by imposing different gauge conditions, up to factor orderings.

The last condition is important and ultimately leads to violations of time reparameterization invariance or covariance of internal-time formulations. The effective constrained system provides gauge transformations that map moment corrections in an evolution generator for one time choice to the moment corrections obtained with a different time choice, including proper time. However, in our model, the time choices we studied explicitly, given by scalar time, cosmological time and proper time, all require different factor orderings of the constraint operator for real evolution generators. Since effective constraints are computed for a given factor ordering of the constraint operator, they do not allow gauge transformations that would change factor ordering corrections. Factor ordering terms therefore generically imply that different time choices lead to different predictions, and time reparameterization invariance of internal-time formulations is broken. The only solution to this important problem is to insist on one specific time choice for all derivations. The only distinguished time choice, in our opinion, is proper time: it refers directly to the time experienced by observers and gives evolution equations that can be used directly in an effective Friedmann equation of cosmological models. Moreover, it is time-reparameterization invariant when compared with other choices of coordinate time, while there are no complete transformations for different choices of internal time.

We have worked entirely at an effective level up to second order in moment corrections, corresponding to a semiclassical approximation to first order in \hbar . This order suffices to demonstrate our claims because differences in quantum corrections between the models are visible at this order. In principle, one can extend the effective expansion to higher orders, but it becomes more involved and is then best done using computational help. We have not considered such an extension in the present paper because the orders we did include already show quite dramatic differences between the models if improper gauge conditions are used, for instance by trying to rewrite a deparameterized model in proper time by using the 1-parameter chain rule.

Our deparameterized models could certainly be formulated with operators acting on a physical Hilbert space without using an effective theory. However, no general method is known that would allow one to compare physical Hilbert spaces based on different deparameterizations, or to introduce proper time at this level. By using an effective formulation, we have gained the advantage of being able to embed all such models within the same constrained system, and to transform their moment corrections by simple changes of gauge conditions. These properties were crucial in our strict definition of proper-time evolution at the quantum level, for which we used effective observables such as invariant moments instead of operators on a physical Hilbert space. Internal-time formulations based on a single physical Hilbert space, as used for instance in loop quantum cosmology, cannot be assumed to give correct moment terms in effective equations, strengthening the results of [6]. Investigations of internal-time formulations of quantum cosmological models with significant quantum fluctuations are therefore likely to be spurious.

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