Time in quantum cosmology

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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 unambiguous 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 different choices of internal time can be compared, and it suggests a new definition of coordinate time in quantum cosmology which is amenable to a notion of time reparameterization invariance. In addition to corrections from moments such as quantum fluctuations, also factor ordering corrections may appear. The latter generically lead to inequivalent internal-time formulations owing to quantization ambiguities.

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I. 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 a phase-space degrees of freedom as a measure of change for other variables [1–9]. 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 [10–12] 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.

The question of covariance in internal-time formulations has rarely been studied, but some results are available [13, 14]. In this paper, we use semiclassical methods developed for effective constraints [15–19] in order to approach this question. We analyze an explicit model which permits (at least) 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 proper-time parameter turns out to be a more complicated step than usually appreciated. Such a parameter is important when one relates 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.

It turns out that covariance in effective Friedmann equations is more involved than has been appreciated in the past. In most 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, and reviewed briefly in the appendix; see for instance [20] 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 expectation-value 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 is therefore violated: Although there is a single constraint operator $\hat{C}$, physical states for effective equations that combine scale-factor dynamics with fluctuation terms are subject to multiple independent constraints of the form $\langle \hat{O}\hat{C} \rangle$. Making sure that time reparameterization invariance, or more generally covariance, is still realized after quantization, or checking under which conditions it may be broken, is then an important task of quantum cosmology.

We 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 internal times 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 evolution in effective equations such that time reparameterization invariance is realized in moment corrections. Our new definition leads to evolution equations with moment corrections which are obtained from those in internal-time 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 time may give rise to different factor orderings. 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. In our specific model, the 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 [13] more specific. However, the new effective evolution introduced here is time reparameterization invariant in the sense that a lapse function can be chosen freely. Quantum evolution remains sensitive to factor-ordering choices, but they are now clearly separate from the choice of time.

II. 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

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

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

We introduce the following canonical variables. (See [21] 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, while T 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 any physical meaning or to be measurable. This property 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 global internal times. The variable T, in fact, does have an advantage compared with $\tilde{\phi}$ because the energy density associated with this degree of freedom 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. Using a scalar time in quantum cosmology goes back to [22], while internal times similar to T have been used for instance in [23–25].

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 to avoid distractions from the important terms. We introduce

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

and its canonical conjugate 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

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

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

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

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

III. DEPARAMETERIZATION

We first deparameterize the model in two different ways, using the global internal times ϕ and T, respectively. A third choice introduces a new time variable as a combination of ϕ and p_ϕ. We begin with the more familiar choice ϕ, solving $C = 0$ for the momentum

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

A. Scalar time

In this section, we quantize the model after deparameterization, so that there is an operator $\hat{p}_\phi$ 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 [26, 27] then allow us to compute an effective Hamiltonian by formally expanding the expectation value

$$\begin{aligned} H_\phi &:= \langle p_\phi(\hat{V}, \hat{H}, \hat{\Lambda})\rangle = \langle p_\phi(V + (\hat{V} - V), H + (\hat{H} - H), \Lambda + (\hat{\Lambda} - \Lambda))\rangle \\ &= p_\phi(V, H, \Lambda) + \sum_{a_1, a_2, a_3 = 2}^{\infty} \frac{1}{a_1! a_2! a_3!} \frac{\partial^{a_1 + a_2 + a_3} p_\phi(V, H, \Lambda)}{\partial V^{a_1} \partial H^{a_2} \partial \Lambda^{a_3}} \Delta(V^{a_1} H^{a_2} \Lambda^{a_3}) \end{aligned} \tag{10}$$

in $\hat{V} - V$, $\hat{H} - H$ and $\hat{\Lambda} - \Lambda$. (This equation is a generalization of (A3) to three independent variables.)

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

$$\Delta(O_1^{a_1} \cdots O_n^{a_n}) = \langle (\hat{O}_1 - O_1)^{a_1} \cdots (\hat{O}_n - O_n)^{a_n} \rangle_{\mathrm{symm}} \tag{11}$$

(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

$$H_\phi = -V\sqrt{H^2 - \Lambda} - \frac{H}{\sqrt{H^2 - \Lambda}}\Delta(VH) + \frac{1}{2}\frac{V\Lambda}{(H^2 - \Lambda)^{3/2}}\Delta(H^2) \tag{12}$$

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

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

$$\{A,B\}=\frac{\langle[\hat{A},\hat{B}]\rangle}{i\hbar} \tag{13}$$

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 [26, 28], but for small orders it is usually more convenient to compute brackets directly from (13). For instance,

$$\{\Delta(H^2),\Delta(V^2)\} \;=\; 4\Delta(VH)\,, \tag{14}$$
$$\{\Delta(H^2),\Delta(VH)\} \;=\; 2\Delta(H^2)\,, \tag{15}$$
$$\{\Delta(V^2),\Delta(VH)\} \;=\; -2\Delta(V^2)\,. \tag{16}$$

These Poisson brackets give rise to the equations of motion

$$\begin{aligned}\frac{\mathrm{d}V}{\mathrm{d}\phi} \;&=\; \{V,H_\phi\}=\frac{VH}{\sqrt{H^2-\Lambda}}-\frac{\Lambda}{(H^2-\Lambda)^{3/2}}\Delta(VH)+\frac{3}{2}\frac{VH\Lambda}{(H^2-\Lambda)^{3/2}}\Delta(H^2)\\ &\quad+\frac{H}{2(H^2-\Lambda)^{3/2}}\Delta(V\Lambda)-\frac{1}{2}\frac{V(2H^2+\Lambda)}{(H^2-\Lambda)^{5/2}}\Delta(H\Lambda)+\frac{3}{8}\frac{VH}{(H^2-\Lambda)^{5/2}}\Delta(\Lambda^2)\end{aligned} \tag{17}$$

and

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

accompanied by equations of motion for the moments such as

$$\frac{\mathrm{d}\Delta(V^2)}{\mathrm{d}\phi}=2\frac{H}{\sqrt{H^2-\Lambda}}\Delta(V^2)-2\frac{V\Lambda}{(H^2-\Lambda)^{3/2}}\Delta(VH)+\frac{VH}{(H^2-\Lambda)^{3/2}}\Delta(V\Lambda)\,. \tag{19}$$

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 $\mathrm{d}\phi/\mathrm{d}\tau=\{\phi,C\}$. However, within the deparameterized setting, we do not have a quantum-corrected 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

$$h_\phi:=\frac{p_\phi^2}{V}-2\frac{p_\phi}{V^2}\Delta(Vp_\phi)+\frac{p_\phi^2}{V^3}\Delta(V^2)+\frac{1}{V}\Delta(p_\phi^2)\,, \tag{20}$$

leading to

$$\begin{aligned}\frac{\mathrm{d}\phi}{\mathrm{d}\tau} \;&=\; \{\phi,-h_\phi\}=-2\frac{p_\phi}{V}+\frac{2}{V^2}\Delta(Vp_\phi)-\frac{2p_\phi}{V^3}\Delta(V^2) &(21)\\ &=\; 2\sqrt{H^2-\Lambda}+2\frac{\sqrt{H^2-\Lambda}}{V^2}\Delta(V^2)+\frac{2H}{V\sqrt{H^2-\Lambda}}\Delta(VH)-\frac{\Lambda}{(H^2-\Lambda)^{3/2}}\Delta(H^2) &(22)\\ &\quad-\frac{1}{V\sqrt{H^2-\Lambda}}\Delta(V\Lambda)+\frac{H}{(H^2-\Lambda)^{3/2}}\Delta(H\Lambda)-\frac{1}{4}\frac{1}{(H^2-\Lambda)^{3/2}}\Delta(\Lambda^2)+\frac{2}{V^2}\Delta(Vp_\phi)\end{aligned}$$

if we also eliminate $p_\phi=H_\phi$ using (12). We have used $-h_\phi$ in order to align forward motion of ϕ with forward motion of τ. The chain rule then gives the proper-time equations

$$\begin{aligned}\frac{\mathrm{d}V}{\mathrm{d}\tau} &= \frac{\mathrm{d}V}{\mathrm{d}\phi}\frac{\mathrm{d}\phi}{\mathrm{d}\tau} = 2VH + 2\Delta(VH) + 2\frac{VH\Lambda}{(H^2-\Lambda)^2}\Delta(H^2)\\ &\quad -2\frac{Hp_\phi}{V^2\sqrt{H^2-\Lambda}}\Delta(V^2) + 2\frac{H}{V\sqrt{H^2-\Lambda}}\Delta(Vp_\phi)\\ &\quad -\frac{V(H^2+\Lambda)}{(H^2-\Lambda)^2}\Delta(H\Lambda) + \frac{1}{2}\frac{VH}{(H^2-\Lambda)^2}\Delta(\Lambda^2) \end{aligned} \tag{23}$$

and

$$\begin{aligned}\frac{\mathrm{d}H}{\mathrm{d}\tau} &= -2(H^2-\Lambda) - 2\frac{H}{V}\Delta(VH) + \frac{2\Lambda}{H^2-\Lambda}\Delta(H^2)\\ &\quad +2\frac{p_\phi\sqrt{H^2-\Lambda}}{V^3}\Delta(V^2) - 2\frac{\sqrt{H^2-\Lambda}}{V^2}\Delta(Vp_\phi)\\ &\quad +\frac{1}{V}\Delta(V\Lambda) - 2\frac{H}{H^2-\Lambda}\Delta(H\Lambda) + \frac{1}{2}\frac{1}{H^2-\Lambda}\Delta(\Lambda^2)\,. \end{aligned} \tag{24}$$

Alternatively, we could square the deparameterized quantum Hamiltonian (12) and rearrange terms so as to make the expression look like the classical constraint plus moment terms. We obtain

$$\begin{aligned} 0 &= \frac{H_\phi^2}{V} - V^2(H^2-\Lambda) - 2H\Delta(VH) + \frac{V\Lambda}{H^2-\Lambda}\Delta(H^2)\\ &\quad +\Delta(V\Lambda) - \frac{VH}{H^2-\Lambda}\Delta(H\Lambda) + \frac{1}{4}\frac{V}{H^2-\Lambda}\Delta(\Lambda^2) \end{aligned} \tag{25}$$

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

$$\begin{aligned}\frac{\mathrm{d}\phi}{\mathrm{d}\tau} &= -2\frac{H_\phi}{V} = 2\sqrt{H^2-\Lambda} + \frac{2H}{V\sqrt{H^2-\Lambda}}\Delta(VH)\\ &\quad -\frac{\Lambda}{(H^2-\Lambda)^{3/2}}\Delta(H^2) - \frac{1}{V\sqrt{H^2-\Lambda}}\Delta(V\Lambda)\\ &\quad +\frac{H}{(H^2-\Lambda)^{3/2}}\Delta(H\Lambda) - \frac{1}{4}\frac{1}{(H^2-\Lambda)^{3/2}}\Delta(\Lambda^2) \end{aligned} \tag{26}$$

and

$$\begin{aligned}\frac{\mathrm{d}V}{\mathrm{d}\tau} &= 2VH + 2\Delta(VH) + 2\frac{VH\Lambda}{(H^2-\Lambda)^2}\Delta(H^2) \\ &\quad -\frac{V(H^2+\Lambda)}{(H^2-\Lambda)^2}\Delta(H\Lambda) + \frac{1}{2}\frac{VH}{(H^2-\Lambda)^2}\Delta(\Lambda^2)\,, \end{aligned} \tag{27}$$

$$\begin{aligned}\frac{\mathrm{d}H}{\mathrm{d}\tau} &= -2(H^2-\Lambda) - 2\frac{H}{V}\Delta(VH) + \frac{2\Lambda}{H^2-\Lambda}\Delta(H^2)\\ &\quad +\frac{1}{V}\Delta(V\Lambda) - 2\frac{H}{H^2-\Lambda}\Delta(H\Lambda) + \frac{1}{2}\frac{1}{H^2-\Lambda}\Delta(\Lambda^2)\,. \end{aligned} \tag{28}$$

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

As we will discuss in more detail later, the main reason for this ambiguity in the definition of proper-time evolution from internal times is the fact that the original constraint, $\hat{C}$ or $\langle\hat{C}\rangle$, is reformulated when one transitions to internal time. Quantum corrections in the resulting system then are not directly related to quantum effects in $\hat{C}$.

B. Cosmological time

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

$$\Lambda(V, H, p_\phi) = H^2 - \frac{p_\phi^2}{V^2}\,. \tag{29}$$

Its semiclassical quantization gives the Hamiltonian

$$H_T = H^2 - \frac{p_\phi^2}{V^2} + \Delta(H^2) - \frac{3p_\phi^2}{V^4}\Delta(V^2) - \frac{1}{V^2}\Delta(p_\phi^2) + 4\frac{p_\phi}{V^3}\Delta(Vp_\phi)\,, \tag{30}$$

generating equations of motion

$$\frac{\mathrm{d}V}{\mathrm{d}T} = -2H \tag{31}$$

and

$$\frac{\mathrm{d}H}{\mathrm{d}T} = 2\frac{p_\phi^2}{V^3} + 12\frac{p_\phi^2}{V^5}\Delta(V^2) + \frac{2}{V^3}\Delta(p_\phi^2) - 12\frac{p_\phi}{V^4}\Delta(Vp_\phi)\,. \tag{32}$$

We attempt to transform to proper time using

$$\frac{\mathrm{d}T}{\mathrm{d}\tau} = \{T, -C\} = -V\,. \tag{33}$$

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

$$\frac{\mathrm{d}V}{\mathrm{d}\tau} = 2VH \tag{34}$$

and

$$\frac{\mathrm{d}H}{\mathrm{d}\tau} = -2\frac{p_\phi^2}{V^2} - 12\frac{p_\phi^2}{V^4}\Delta(V^2) - \frac{2}{V^2}\Delta(p_\phi^2) + 12\frac{p_\phi}{V^3}\Delta(Vp_\phi) \tag{35}$$

$$\approx\ -2(H^2-\Lambda)-2\Delta(H^2)-6\frac{H^2-\Lambda}{V^2}\Delta(V^2)+4\frac{p_\phi}{V^3}\Delta(Vp_\phi)\,. \tag{36}$$

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.

C. 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 (only) 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

$$C=-VH^2+\frac{p}{V}+V\Lambda=0 \tag{37}$$

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

Proceeding as before, we have the quantum Hamiltonian

$$H_q=V^2(H^2-\Lambda)+(H^2-\Lambda)\Delta(V^2)+4VH\Delta(VH)+V^2\Delta(H^2)-2V\Delta(V\Lambda) \tag{38}$$

and the internal-time evolution equations

$$\begin{aligned}\frac{\mathrm{d}V}{\mathrm{d}q}&=-2V^2H-2H\Delta(V^2)-4V\Delta(VH)\,, \qquad (39)\\ \frac{\mathrm{d}H}{\mathrm{d}q}&=2V(H^2-\Lambda)+4H\Delta(VH)+2V\Delta(H^2)-2\Delta(V\Lambda)\,.\end{aligned}$$

Internal time q is tentatively related to proper time τ by

$$\frac{\mathrm{d}q}{\mathrm{d}\tau}=-\frac{1}{V}\,, \tag{40}$$

and we obtain proper-time equations

$$\begin{aligned}\frac{\mathrm{d}V}{\mathrm{d}\tau}&=2VH+2\frac{H}{V}\Delta(V^2)+4\Delta(VH)\,, \qquad (41)\\ \frac{\mathrm{d}H}{\mathrm{d}\tau}&=-2(H^2-\Lambda)-4\frac{H}{V}\Delta(VH)-2\Delta(H^2)+\frac{2}{V}\Delta(V\Lambda)\end{aligned}$$

which agree with none of the previous versions.

IV. 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 $\mathrm{d}/\mathrm{d}\tau=\{\cdot,C\}$ 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, at first sight, 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.

A. Effective constraints

Using the canonical effective description of [15, 16], 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

$$C_1:=\langle\hat{C}\rangle=0 \tag{42}$$

is a constraint, but also all expressions of the form

$$C_f:=\langle(\hat{f}-f)\hat{C}\rangle=0 \tag{43}$$

where f is an arbitrary classical phase-space function and $\hat{f}$ its (Weyl-ordered) quantization. For f not a constant, 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 like expectation values of Hamiltonians in the deparameterized models, the effective constraints can be expanded in moments. We have

$$C_1(O_1,\ldots,O_n,\Delta(\cdot)) = C(O_1,\ldots,O_n) + \sum_{a_1,\ldots,a_n} \frac{1}{a_1!\cdots a_n!} \frac{\partial^{a_1+\cdots+a_n} C(O_1,\ldots,O_n)}{\partial O_1^{a_1}\cdots\partial O_n^{a_n}} \Delta(O^{a_1}\cdots O^{a_n}) \tag{44}$$

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.

B. 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

$$\begin{aligned}
C_1 &= -VH^2 + \frac{p_\phi^2}{V} + V\Lambda + \frac{p_\phi^2}{V^3}\Delta(V^2) - 2H\Delta(VH) - V\Delta(H^2) \\
&\quad + \frac{1}{V}\Delta(p_\phi^2) - 2\frac{p_\phi}{V^2}\Delta(Vp_\phi) + \Delta(V\Lambda)\,,
\end{aligned} \tag{45}$$

$$\begin{aligned}
C_V &= -\left(H^2 + \frac{p_\phi^2}{V^2} - \Lambda\right)\Delta(V^2) - 2VH\left(\Delta(VH) - \frac{1}{2}i\hbar\right) \\
&\quad + 2\frac{p_\phi}{V}\Delta(Vp_\phi) + V\Delta(V\Lambda)\,,
\end{aligned} \tag{46}$$

$$\begin{aligned}
C_H &= -2VH\Delta(H^2) - \left(H^2 + \frac{p_\phi^2}{V^2} - \Lambda\right)\left(\Delta(VH) + \frac{1}{2}i\hbar\right) \\
&\quad + 2\frac{p_\phi}{V}\Delta(Hp_\phi) + V\Delta(H\Lambda)\,,
\end{aligned} \tag{47}$$

$$\begin{aligned}
C_\phi &= -\left(H^2 + \frac{p_\phi^2}{V^2} - \Lambda\right)\Delta(V\phi) - 2VH\Delta(H\phi) \\
&\quad + 2\frac{p_\phi}{V}\left(\Delta(\phi p_\phi) + \frac{1}{2}i\hbar\right) + V\Delta(\phi\Lambda)\,,
\end{aligned} \tag{48}$$

$$C_{p_\phi} = -\left(H^2 + \frac{p_\phi^2}{V^2} - \Lambda\right)\Delta(Vp_\phi) - 2VH\Delta(Hp_\phi) + 2\frac{p_\phi}{V}\Delta(p_\phi^2) + V\Delta(p_\phi\Lambda)\,, \tag{49}$$

$$\begin{aligned}
C_T &= -\left(H^2 + \frac{p_\phi^2}{V^2} - \Lambda\right)\Delta(VT) - 2VH\Delta(HT) + 2\frac{p_\phi}{V}\Delta(p_\phi T) \\
&\quad + V\left(\Delta(\Lambda T) + \frac{1}{2}i\hbar\right)\,,
\end{aligned} \tag{50}$$

$$C_\Lambda \;=\; -\left(H^2+\frac{p_\phi^2}{V^2}-\Lambda\right)\Delta(V\Lambda)-2VH\Delta(H\Lambda)+2\frac{p_\phi}{V}\Delta(p_\phi\Lambda)+V\Delta(\Lambda^2)\,. \tag{51}$$

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 [15, 16], 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 [15, 16], it has been shown that the effective constraints form a first-class system. Therefore, they generate gauge transformations. (For this property, it is important that we do *not* symmetrize $\hat{f}\hat{C}$ in the definition of C_f.) 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 [29] 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.

C. 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

$$\Delta(\phi^2)=\Delta(V\phi)=\Delta(H\phi)=\Delta(\phi T)=\Delta(\phi\Lambda)=0 \tag{52}$$

which, as shown in [17, 18], 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

$$\Delta(\phi p_\phi)=-\frac{1}{2}i\hbar \tag{53}$$

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

$$\Delta(\phi^2)\Delta(p_\phi)^2-\Delta(\phi p_\phi)^2\geq\frac{\hbar^2}{4} \tag{54}$$

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

1. *Scalar time*

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

$$\Delta(Vp_\phi)=\frac{1}{2}\frac{V}{p_\phi}\left(\left(H^2+\frac{p_\phi^2}{V^2}-\Lambda\right)\Delta(V^2)+2VH\left(\Delta(VH)-\frac{1}{2}i\hbar\right)-V\Delta(V\Lambda)\right)\;; \tag{55}$$

from $C_H=0$,

$$\Delta(Hp_\phi)=\frac{1}{2}\frac{V}{p_\phi}\left(2VH\Delta(H^2)+\left(H^2+\frac{p_\phi^2}{V^2}-\Lambda\right)\left(\Delta(VH)+\frac{1}{2}i\hbar\right)-V\Delta(H\Lambda)\right)\;; \tag{56}$$

from $C_\Lambda=0$,

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

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

$$\Delta(p_\phi^2)\;=\;\frac{1}{2}\frac{V}{p_\phi}\left(\left(H^2+\frac{p_\phi^2}{V^2}-\Lambda\right)\Delta(Vp_\phi)+2VH\Delta(Hp_\phi)-V\Delta(p_\phi\Lambda)\right) \tag{58}$$

$$= \frac{1}{4}\frac{V^2}{p_\phi^2}\left(H^2+\frac{p_\phi^2}{V^2}-\Lambda\right)^2\Delta(V^2)+\frac{V^4H^2}{p_\phi^2}\Delta(H^2)+\frac{V^3H}{p_\phi^2}\left(H^2+\frac{p_\phi^2}{V^2}-\Lambda\right)\Delta(VH)$$
$$-\frac{1}{2}\frac{V^3}{p_\phi^2}\left(H^2+\frac{p_\phi^2}{V^2}-\Lambda\right)\Delta(V\Lambda)-\frac{V^4H}{p_\phi^2}\Delta(H\Lambda)+\frac{1}{4}\frac{V^4}{p_\phi^2}\Delta(\Lambda^2)\,. \tag{59}$$

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 [30] 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 [18, 31], one can check that, in the present example, the unique generator respecting the gauge-fixing conditions is of the form

$$NC = \frac{1}{2p_\phi}\left((VC)_1 - \frac{1}{2p_\phi}(VC)_{p_\phi} - \frac{1}{2p_\phi}\frac{\partial p_\phi}{\partial V}(VC)_V - \frac{1}{2p_\phi}\frac{\partial p_\phi}{\partial H}(VC)_H - \frac{1}{2p_\phi}\frac{\partial p_\phi}{\partial \Lambda}(VC)_\Lambda - \frac{1}{2p_\phi}\frac{\partial p_\phi}{\partial T}(VC)_T\right) \tag{60}$$

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,

$$(VC)_1 = \langle (V + (\hat{V} - V))\hat{C}\rangle = VC_1 + C_V \tag{61}$$

and

$$(VC)_V = \langle (\hat{V} - V)(V + (\hat{V} - V))\hat{C}\rangle = VC_V + \Delta(V^2)C_1 \tag{62}$$

or, in general,

$$(AC)_B = \langle (\hat{B} - B)(A + (\hat{A} - A))\hat{C}\rangle$$
$$= AC_B + \left(\Delta(AB) - \frac{1}{2}\langle[\hat{A},\hat{B}]\rangle\right)C_1\,. \tag{63}$$

For our present purposes, it suffices to justify the combination (60) of constraints by confirming that the resulting generator

$$NC = \frac{p_\phi - V\sqrt{H^2-\Lambda}}{2p_\phi}\left(p_\phi + V\sqrt{H^2-\Lambda}\right) + \frac{H}{\sqrt{H^2-\Lambda}}\Delta(VH) - \frac{1}{2}\frac{V\Lambda}{(H^2-\Lambda)^{3/2}}\Delta(H^2)$$
$$-\frac{1}{2\sqrt{H^2-\Lambda}}\Delta(V\Lambda) + \frac{1}{2}\frac{VH}{(H^2-\Lambda)^{3/2}}\Delta(H\Lambda) - \frac{1}{8}\frac{V}{(H^2-\Lambda)^{3/2}}\Delta(\Lambda^2) \tag{64}$$

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 (12). We therefore confirm that deparemeterization can be performed before or after quantization, with equivalent results.

2. Cosmological time

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

$$\Delta(T^2) = \Delta(VT) = \Delta(HT) = \Delta(\phi T) = \Delta(p_\phi T) = 0 \tag{65}$$

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,

$$\begin{aligned}\left(V^{-1}C'\right)_1 &= -H^2 + \frac{p_\phi^2}{V^2} + \Lambda - \Delta(H^2) + 3\frac{p_\phi^2}{V^4}\Delta(V^2) \\ &\quad -4\frac{p_\phi}{V^3}\Delta(Vp_\phi) + \frac{1}{V^2}\Delta(p_\phi^2)\end{aligned} \tag{66}$$

contains no such moments. Solving $(V^{-1}C')_1 = 0$ for $\Lambda = H_T$ gives an expression for the T-Hamiltonian identical with (30).

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

$$\hat{V}\hat{H}^2 = \frac{1}{3}(\hat{V}\hat{H}^2+\hat{H}\hat{V}\hat{H}+\hat{H}^2\hat{V})-i\hbar\hat{H} = (\hat{V}\hat{H}^2)_{\rm Weyl}-i\hbar\hat{H}\,. \tag{67}$$

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

$$\begin{aligned}\left(V^{-1}C'\right)_1 &= \langle (V^{-1} - V^{-2}(\hat{V}-V))(\hat{C} - i\hbar\hat{H})\rangle \\ &= \frac{C_1}{V} - \frac{C_V - i\hbar VH}{V^2}\end{aligned} \tag{68}$$

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

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. 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 in this sense.

D. Non-covariance

Using effective constraints, we have rederived the deparameterized Hamiltonians (12) and (30) for our model with two different choices of internal time. The agreement with derivations in deparameterized models in the preceding Sec. III 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 [18].) 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. III would be equivalent to each other. However, in our explicit example, covariance is broken by factor ordering corrections, which exist whenever the momenta of two internal times appear in the constraint with different phase-space dependent factors. Nevertheless, this result, which we consider to be rather important, cannot explain the mismatch of proper-time evolutions we found in Sec. III 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 proper-time evolution from internal-time evolution required an expression for $\mathrm{d}\phi/\mathrm{d}\tau$ or $\mathrm{d}T/\mathrm{d}\tau$. 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. The common reference to the chain rule, transforming from an internal time to proper time, is meaningless in this context of multiple constraints. The 1-parameter chain rule $\mathrm{d}/\mathrm{d}\tau = (\mathrm{d}\phi/\mathrm{d}\tau)\mathrm{d}/\mathrm{d}\phi$ 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.

E. Coordinate time

There is a way to obtain a notion of coordinate-time evolution from the effective constraints. A time coordinate 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 observables of this subset of constraints.

This approach to introducing time in systems with a Hamiltonian constraint is new, and therefore requires several technical developments which will be given first. In particular, there are subtleties in defining a suitable set of variables which are invariant under gauge transformations generated only by a subset of constraints which do not form an ideal with respect to the Poisson bracket. Here, we are interested in invariance under the flow of C_f with f a basic operator up to terms that vanish when the remaining constraint, C_1, is imposed. These variables are not invariant under the remaining flow of C_1, which we will then be able to interpret as time evolution as in an effective Friedmann equation. While the Poisson bracket of a complete Dirac observable of all the effective constraint would again be a Dirac observable, thanks to the Jacobi identity, the Poisson bracket of two variables invariant under gauge transformations generated by the C_f is not guaranteed to be invariant under the same transformations. However, since we are interested in partial gauge invariance up to terms proportional to C_1, there is the freedom of adding terms proportional to C_1 to candidates for partially invariant quantities. As we will demonstrate, for each variable it is possible to add a term proportional to C_1 such that Poisson brackets of any pair of these partially invariant quantities are partially invariant in the same sense.

In this process, we will notice some unexpected Poisson brackets, which differ from what one would expect for kinematical expectation values or moments. For instance, for partially invariant moments, the volume fluctuation does not Poisson commute with the covariance of the volume and p_ϕ, in contrast to what one would expect if p_ϕ is independent of the volume. Or, partially invariant expectation values may have non-vanishing Poisson brackets with partially invariant moments, while such brackets would always be zero for kinematical expectation values and (Weyl-ordered) moments. We will explain these unexpected results quantitatively by observing the fact that partially implementing the constraints leads one toward physical states, on which p_ϕ is no longer independent of the volume by virtue of the constraint.

Having derived a set of partially invariant variables closed under taking Poisson brackets, we will obtain reduced constraints, defined as the remaining constraint C_1 expressed purely in terms of partially gauge-invariant variables. At this point, we will be dealing with systems subject to a single effective constraint, which is closer to classical singly-constrained systems (except that we still have partially invariant moments as independent degrees of freedom). This property makes it easier to interpret the reduced constraint as generating time evolution with respect to coordinate time, just as the classical Hamiltonian constraint generates the Friedmann and Raychaudhuri equations and thereby time evolution. We will find a remaining trace of a dependence of choosing an internal time, which in this approach comes about because sets of partially invariant variables closed under taking Poisson brackets are not unique even with this closure condition. In order to make variables partially invariant, one combines expectation values and moments such that the partial gauge transformations cancel out. There is a choice involved in how one chooses such combinations, which can be formulated as whether one adds suitable ϕ-moments or suitable T-moments or, in general, moments of a fixed kinematical variable. To some degree, we thus encounter the internal-time problem in disguise, even though we will be developing a coordinate-time framework. However, in contrast to strict internal-time treatments as in our previous examples, different choices now lead to mutually consistent results, which will lead us to the proposal of a new formulation of coordinate time in effective constrained systems at the end of this section.

1. Partially reduced variables

Up to terms of higher order in $\hbar$ including products of second-order moments, as always in this paper, the variables

$$\mathcal{V}_1 = V - \frac{VH}{p_\phi}\Delta(V\phi) - \frac{V^2}{p_\phi}\Delta(H\phi) + \frac{V^3\Lambda}{2p_\phi^2}\Delta(\phi^2) \quad (69)$$

$$\mathcal{H}_1 = H + 2\frac{VH}{p_\phi}\Delta(H\phi) - \frac{V}{p_\phi}\Delta(\phi\Lambda) + H\Delta(\phi^2) \quad (70)$$

as well as

$$\Delta_1(\mathcal{V}^2) = \Delta(V^2) - 2\frac{V^2H}{p_\phi}\Delta(V\phi) + \frac{V^4H^2}{p_\phi^2}\Delta(\phi^2) \quad (71)$$

$$\Delta_1(\mathcal{V}\mathcal{H}) = \Delta(VH) + \frac{p_\phi}{V}\Delta(V\phi) - \frac{V^2H}{p_\phi}\Delta(H\phi) - HV\Delta(\phi^2)\,, \quad (72)$$

$$\Delta_1(\mathcal{H}^2) = \Delta(H^2) + 2\frac{p_\phi}{V}\Delta(H\phi) + \frac{p_\phi^2}{V^2}\Delta(\phi^2)\,, \quad (73)$$

$$\Delta_1(\mathcal{V}p_\phi) = \Delta(Vp_\phi) - \frac{V^2H}{p_\phi}\Delta(\phi p_\phi)\,, \quad (74)$$

$$\Delta_1(\mathcal{H}p_\phi) = \Delta(Hp_\phi) + \frac{p_\phi}{V}\Delta(\phi p_\phi)\,, \quad (75)$$

$$\Delta_1(\mathcal{V}\Lambda) = \Delta(V\Lambda) - \frac{HV^2}{p_\phi}\Delta(\phi\Lambda)\,, \quad (76)$$

$$\Delta_1(\mathcal{H}\Lambda) = \Delta(H\Lambda) + \frac{p_\phi}{V}\Delta_1(\phi\Lambda) \quad (77)$$

are invariant (up to terms proportional to C_1) under the flow generated by the constraints C_f with f a basic phase-space variable. Moreover, p_ϕ, Λ, $\Delta(p_\phi^2)$, $\Delta(p_\phi\Lambda)$ and $\Delta(\Lambda^2)$ are invariant.

Note that $\Delta_1(\mathcal{V}p_\phi)$ in (74) and $\Delta_1(\mathcal{H}p_\phi)$ in (75) are real even if ϕ is used as internal time because the non-zero imaginary parts of $\Delta(Vp_\phi)$ or $\Delta(Hp_\phi)$ and $\Delta(\phi p_\phi)$, according to (55) or (56) and (53), cancel out completely. It is also possible to understand the additional terms in (74) and (75) as a consequence of the fact that p_ϕ is not independent of V and H after one solves constraints. Using the relationship $p_\phi = -V\sqrt{H^2-\Lambda} + O(\Delta)$ and calculating to semiclassical order, we then expect to have

$$\begin{aligned}\Delta(\mathcal{V}p_\phi) &= \frac{1}{2}\left\langle \widehat{\Delta V}\widehat{\Delta p_\phi} + \widehat{\Delta p_\phi}\widehat{\Delta V}\right\rangle = \left\langle \widehat{\Delta V}\widehat{\Delta p_\phi} - \tfrac{1}{2}[\hat{V},\hat{p}_\phi]\right\rangle \\ &= \left\langle \widehat{\Delta V}\widehat{\Delta p_\phi}\rangle + \tfrac{1}{2}i\hbar\langle\widehat{\partial p_\phi/\partial H}\right\rangle \\ &= \Delta(Vp_\phi) + \frac{1}{2}i\hbar\frac{\partial p_\phi}{\partial H} + O(\hbar\Delta) \\ &= \Delta(Vp_\phi) - \frac{\partial p_\phi}{\partial H}\Delta(\phi p_\phi)\,. \end{aligned} \quad (78)$$

Here, we identify partially invariant moments, such as $\Delta(\mathcal{V}p_\phi)$, with moments on a physical Hilbert space, while the non-invariant $\Delta(Vp_\phi)$ corresponds to a moment on the kinematical Hilbert space on which $\hat{V}$ and $\hat{p}_\phi$ commute. The result agrees with (74), and the same can be shown for (75).

The remaining partially invariant moments, by contrast, receive non-zero real contributions from moments including ϕ, which all vanish in the gauge (52) leading to ϕ as internal time, but only in this gauge. In this gauge of a formulation deparameterized by internal time ϕ, the partially reduced variables are equal to the real parts of 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 (65), there are additional non-zero moments compared with the simple kinematical expressions V, H, $\Delta(V^2)$, $\Delta(VH)$, $\Delta(H^2)$, $\Delta(Vp_\phi)$, $\Delta(Hp_\phi)$, $\Delta(V\Lambda)$ and $\Delta(H\Lambda)$. If one analyzes a model using different internal times, such as ϕ and T in the present case, one therefore should 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. Such a relationship can be seen only if one allows for different internal times in one setting, rather than deparameterizing with a single choice of internal time.

2. Poisson brackets

The combinations of expectation values and moments in (69) and (70) are invariant under gauge transformations generated by effective constraints C_f with f linear in basic variables, up to second-order moments and terms proportional to C_1. For instance,

$$\begin{aligned}\{\mathcal{V}, C_V\} &= -C_\phi - \frac{V^2}{p_\phi}\left(H^2 - \frac{p_\phi^2}{V^2} - \Lambda\right)\Delta(V\phi) + O(\Delta^2) \\ &= -C_\phi + \frac{V}{p_\phi}\Delta(V\phi)C_1 + O(\Delta^2)\,. \end{aligned} \quad (79)$$

Invariance up to terms proportional to C_1 (without invariance under $\{\cdot, C_1\}$) is suitable for the purpose of deriving proper-time evolution from an effective constraint C_1, but it implies some subtleties. In particular, the variables $\mathcal{H}_1$ and $\mathcal{V}_1$ are not canonically conjugate, and their Poisson bracket is not even invariant under the flows generated by C_f even though $\mathcal{H}_1$ and $\mathcal{V}_1$ are invariant (up to terms proportional to C_1). The Jacobi identity ensures that

$$\{\{\mathcal{H}_1, \mathcal{V}_1\}, C_f\} = \{\{\mathcal{V}_1, C_f\}, \mathcal{H}_1\} - \{\{\mathcal{H}_1, C_f\}, \mathcal{V}_1\} \quad (80)$$

is zero on-shell, up to terms proportional to Poisson brackets of C_1 with $\mathcal{H}_1$ or $\mathcal{V}_1$, but the latter are not proportional to constraints because we have not imposed invariance under the flow generated by C_1. In fact, a direct calculation shows that

$$\{\mathcal{H}_1,\mathcal{V}_1\} = 1-\frac{H}{p_\phi}\Delta(V\phi)+\frac{V^2}{p_\phi^2}\left(-2H^2+\frac{p_\phi^2}{V^2}+\frac{3}{2}\Lambda\right)\Delta(\phi^2)\,. \tag{81}$$

a. Basic expectation values: In order to obtain a canonical pair, we add suitable moment terms to $\mathcal{H}_1$ and $\mathcal{V}_1$ which are proportional to C_1, such that $\mathcal{H} = \mathcal{H}_1+\Delta_{\mathcal{H}}C_1$ and $\mathcal{V}=\mathcal{V}_1+\Delta_{\mathcal{V}}C_1$ are canonically conjugate. The new variables then have a Poisson bracket given by

$$\{\mathcal{H},\mathcal{V}\} = \{\mathcal{H}_1,\mathcal{V}_1\}+\Delta_{\mathcal{H}}\{C_1,\mathcal{V}_1\}+\Delta_{\mathcal{V}}\{\mathcal{H}_1,C_1\}+O(C_1)\,. \tag{82}$$

Given (81), all terms not constant or proportional to C_1 cancel out if

$$-2VH\Delta_{\mathcal{H}}-2(H^2-\Lambda)\Delta_{\mathcal{V}} = \frac{H}{p_\phi}\Delta(V\phi)+\frac{V^2}{p_\phi^2}\left(H^2-\frac{1}{2}\Lambda\right)\Delta(\phi^2)\,. \tag{83}$$

If we choose $\Delta_{\mathcal{H}}=0$, we have

$$\Delta_{\mathcal{V}} = -\frac{H}{2p_\phi(H^2-\Lambda)}\Delta(V\phi)-\frac{V^2}{2p_\phi^2}\frac{H^2-\frac{1}{2}\Lambda}{H^2-\Lambda}\Delta(\phi^2) \tag{84}$$

and therefore

$$\mathcal{H} = \mathcal{H}_1 = H+2\frac{VH}{p_\phi}\Delta(H\phi)-\frac{V}{p_\phi}\Delta(\phi\Lambda)+H\Delta(\phi^2) \tag{85}$$

$$\begin{aligned}\mathcal{V} &= V-\frac{VH}{2p_\phi(H^2-\Lambda)}\left(H^2+\frac{p_\phi^2}{V^2}-\Lambda\right)\Delta(V\phi)-\frac{V^2}{p_\phi}\Delta(H\phi)\\ &\quad+\frac{V^3}{2p_\phi^2(H^2-\Lambda)}\left(H^2\left(H^2-\frac{p_\phi^2}{V^2}\right)-\frac{1}{2}\Lambda\left(H^2-\frac{p_\phi^2}{V^2}+\Lambda\right)\right)\Delta(\phi^2)\,.\end{aligned} \tag{86}$$

Up to second-order moments and terms proportional to C_1, these variables are indeed canonically conjugate:

$$\begin{aligned}\{\mathcal{H},\mathcal{V}\} &= 1-\frac{H}{2p_\phi(H^2-\Lambda)}\left(H^2-\frac{p_\phi^2}{V^2}-\Lambda\right)\Delta(V\phi)\\ &\quad+\frac{V^2}{2p_\phi^2(H^2-\Lambda)}\left(H^2+\frac{3}{2}\Lambda\right)\left(H^2-\frac{p_\phi^2}{V^2}-\Lambda\right)\Delta(\phi^2)\\ &= 1+O(C_1,\Delta^2)\,.\end{aligned} \tag{87}$$

b. Moments: A different issue arises for some of the moments. A straightforward calculation shows that the Poisson brackets

$$\{\Delta_1(\mathcal{V}^2),\Delta_1(\mathcal{V}\mathcal{H}\} = -2\Delta_1(\mathcal{V}\mathcal{H}) \tag{88}$$

$$\{\Delta_1(\mathcal{V}^2),\Delta_1(\mathcal{H}^2)\} = -4\Delta_1(\mathcal{V}\mathcal{H}) \tag{89}$$

$$\{\Delta_1(\mathcal{V}\mathcal{H}),\Delta_1(\mathcal{H}^2)\} = -2\Delta_1(\mathcal{H})^2) \tag{90}$$

are just as expected for a canonical pair $(\mathcal{V},\mathcal{H})$. However, when moments including p_ϕ appear, the situation is different: We have

$$\begin{aligned}\{\Delta_1(\mathcal{V}^2),\Delta_1(\mathcal{V}p_\phi)\} &= -2\frac{\mathcal{V}^2\mathcal{H}}{p_\phi}\Delta_1(\mathcal{V}^2) = -2\frac{\partial p_\phi}{\partial\mathcal{H}}\Delta_1(\mathcal{V}^2)\\ \{\Delta_1(\mathcal{V}\mathcal{H}),\Delta_1(\mathcal{V}p_\phi)\} &= \Delta_1(\mathcal{V}p_\phi)+\frac{p_\phi}{\mathcal{V}}\Delta_1(\mathcal{V}^2)-\frac{\mathcal{V}^2\mathcal{H}}{p_\phi}\Delta_1(\mathcal{V}\mathcal{H})\end{aligned} \tag{91}$$

$$= \Delta_1(\mathcal{V}p_\phi) + \frac{\partial p_\phi}{\partial \mathcal{V}}\Delta_1(\mathcal{V}^2) - \frac{\partial p_\phi}{\partial \mathcal{H}}\Delta_1(\mathcal{V}\mathcal{H}) \tag{92}$$

$$\{\Delta_1(\mathcal{H}^2), \Delta_1(\mathcal{V}p_\phi)\} = 2\Delta_1(\mathcal{H}p_\phi) + 2\frac{p_\phi}{\mathcal{V}}\Delta_1(\mathcal{H}\mathcal{V}) = 2\Delta_1(\mathcal{H}p_\phi) + 2\frac{\partial p_\phi}{\partial \mathcal{V}}\Delta_1(\mathcal{H}\mathcal{V})\,. \tag{93}$$

At first sight, the moments on the right-hand sides not including p_ϕ are unexpected, if one thinks of p_ϕ as a variable independent of $\mathcal{V}$ and $\mathcal{H}$. However, since we have partially solved the constraints, p_ϕ is no longer independent, which explains why all coefficients of the initially questionable terms can be interpreted as partial derivatives of $p_\phi = -\mathcal{V}\sqrt{\mathcal{H}^2 - \Lambda}$ solving the constraint. (In our calculations to first order in moments, moment terms in p_ϕ are not relevant for the above expressions.) An operator calculation then shows that the Poisson brackets with $\Delta_1(\mathcal{V}p_\phi)$ are indeed correct. For instance, we confirm the last bracket above by calculating

$$[\widehat{\Delta H}^2, \widehat{\Delta V}\widehat{\Delta p_\phi}] = \widehat{\Delta H}\widehat{\Delta V}[\widehat{\Delta H}, \widehat{\Delta p_\phi}] + \widehat{\Delta H}[\widehat{\Delta H}, \widehat{\Delta V}]\widehat{\Delta p_\phi} + [\widehat{\Delta H}, \widehat{\Delta V}]\widehat{\Delta p_\phi}\widehat{\Delta H} + \widehat{\Delta V}[\widehat{\Delta H}, \widehat{\Delta p_\phi}]\widehat{\Delta H} \tag{94}$$

$$= \widehat{\Delta H}\widehat{\Delta p_\phi} + \widehat{\Delta p_\phi}\widehat{\Delta H} + (\widehat{\Delta H}\widehat{\Delta V} + \widehat{\Delta V}\widehat{\Delta H})[\hat{H}, \hat{p}_\phi] + \widehat{\Delta V}[[\hat{H}, \hat{p}_\phi], \hat{H}] \tag{95}$$

for $\widehat{\Delta O} := \hat{O} - \langle\hat{O}\rangle$ for any operator $\hat{O}$. We have already used the fact that $[\widehat{\Delta O_1}, \widehat{\Delta O_2}] = [\hat{O}_1, \hat{O}_2]$. The last term in (95), a double commutator, can be ignored because it is at least of the order of $\hbar^2$. Moreover, to this order we can write $[\hat{H}, \hat{p}_\phi] = i\hbar\widehat{\partial p_\phi/\partial V}$, ignoring ordering terms because they would again be of the order of $\hbar^2$. Taking an expectation value of (95),

$$\langle[\widehat{\Delta H}^2, \widehat{\Delta V}\widehat{\Delta p_\phi}]\rangle = 2\Delta(Hp_\phi) + 2\Delta(VH)\frac{\partial p_\phi}{\partial V} + O(\Delta^2) \tag{96}$$

then confirms that (93) is as it should be expected. A similar calculation confirms the remaining brackets with $\Delta_1(\mathcal{V}p_\phi)$, as well as

$$\{\Delta_1(\mathcal{V}^2), \Delta_1(\mathcal{H}p_\phi)\} = -2\Delta_1(\mathcal{V}p_\phi) - 2\frac{\partial p_\phi}{\partial \mathcal{H}}\Delta_1(\mathcal{V}\mathcal{H}) \tag{97}$$

$$\{\Delta_1(\mathcal{V}\mathcal{H}), \Delta_1(\mathcal{H}p_\phi) = -\Delta_1(\mathcal{H}p_\phi) + \frac{\partial p_\phi}{\partial \mathcal{V}}\Delta_1(\mathcal{V}\mathcal{H}) - \frac{\partial p_\phi}{\partial \mathcal{H}}\Delta_1(\mathcal{H}^2) \tag{98}$$

$$\{\Delta_1(\mathcal{H}^2), \Delta_1(\mathcal{H}p_\phi)\} = 2\frac{\partial p_\phi}{\partial \mathcal{V}}\Delta_1(\mathcal{H}^2) \tag{99}$$

and

$$\{\Delta_1(\mathcal{V}^2), \Delta(p_\phi^2)\} = -4\frac{\partial p_\phi}{\partial \mathcal{H}}\Delta_1(\mathcal{V}p_\phi) \tag{100}$$

$$\{\Delta_1(\mathcal{H}^2), \Delta(p_\phi^2)\} = 4\frac{\partial p_\phi}{\partial \mathcal{V}}\Delta_1(\mathcal{H}p_\phi)\,. \tag{101}$$

c. Expectation values and moments: Poisson brackets between a basic expectation value and any (Weyl-ordered, central) moment vanish on the kinematical Hilbert space. Reassuringly, a direct calculation indeed shows that

$$\{\mathcal{V}, \Delta_1(\mathcal{V}^2)\} = 0 = \{\mathcal{H}, \Delta_1(\mathcal{V}^2)\}\,. \tag{102}$$

However, we also obtain

$$\{\mathcal{V}, \Delta_1(\mathcal{V}\mathcal{H})\} = \frac{\mathcal{V}\mathcal{H}}{p_\phi}\Delta_1(\mathcal{V}\phi) - \frac{\mathcal{V}^3\mathcal{H}^2}{p_\phi^2}\Delta(\phi^2) \tag{103}$$

$$\{\mathcal{H}, \Delta_1(\mathcal{V}\mathcal{H})\} = -\frac{p_\phi}{\mathcal{V}^2}\Delta_1(\mathcal{V}\phi) + \mathcal{H}\Delta(\phi^2) \tag{104}$$

$$\{\mathcal{V}, \Delta_1(\mathcal{H}^2)\} = 2\frac{\mathcal{V}\mathcal{H}}{p_\phi}\Delta_1(\mathcal{H}\phi) + 2\mathcal{H}\Delta(\phi^2) \tag{105}$$

$$\{\mathcal{H}, \Delta_1(\mathcal{H}^2)\} = -2\frac{p_\phi}{\mathcal{V}^2}\Delta_1(\mathcal{H}\phi) - 2\frac{p_\phi^2}{\mathcal{V}^3}\Delta(\phi^2) \tag{106}$$

$$\{\mathcal{V}, \Delta_1(\mathcal{V}p_\phi)\} = -\frac{\mathcal{V}\mathcal{H}}{p_\phi}\Delta_1(\mathcal{V}^2) - \frac{\mathcal{V}^2}{p_\phi}\Delta_1(\mathcal{V}\mathcal{H}) \tag{107}$$

$$\{\mathcal{H}, \Delta_1(\mathcal{V}p_\phi)\} = -2\frac{p_\phi}{\mathcal{V}^2}\Delta_1(\mathcal{V}^2) + \frac{2}{\mathcal{V}}\Delta_1(\mathcal{V}p_\phi) \tag{108}$$

$$\{\mathcal{V}, \Delta_1(\mathcal{H}p_\phi)\} = -\frac{\mathcal{V}^2}{p_\phi}\Delta_1(\mathcal{H}^2) - \frac{\mathcal{V}\mathcal{H}}{p_\phi}\Delta_1(\mathcal{V}\mathcal{H}) + \frac{\mathcal{V}\mathcal{H}}{p_\phi}\Delta(\phi p_\phi) \tag{109}$$

$$\{\mathcal{H}, \Delta_1(\mathcal{H}p_\phi)\} = -2\frac{p_\phi}{\mathcal{V}^2}\Delta_1(\mathcal{V}\mathcal{H}) + \frac{2}{\mathcal{V}}\Delta_1(\mathcal{H}p_\phi) - \frac{p_\phi}{\mathcal{V}^2}\Delta(\phi p_\phi) \tag{110}$$

$$\{\mathcal{V}, \Delta(p_\phi^2)\} = -2\frac{\mathcal{V}\mathcal{H}}{p_\phi}\Delta_1(\mathcal{V}p_\phi) - 2\frac{\mathcal{V}^2}{p_\phi}\Delta_1(\mathcal{H}p_\phi) \tag{111}$$

$$\{\mathcal{H},\Delta(p_\phi^2)\} \;=\; -4\frac{p_\phi}{\mathcal{V}^2}\Delta_1(\mathcal{V}p_\phi)+\frac{4}{\mathcal{V}}\Delta(p_\phi^2)\,. \tag{112}$$

In order to understand these non-zero results, we have to combine the two lessons learned for Poisson brackets of partially invariant expectation values and moments. As before, we can redefine the moments by adding terms proportional to C_1, leaving $\mathcal{V}$ and $\mathcal{H}$ unchanged to ensure that $\{\mathcal{V},\mathcal{H}\}=1$ is still respected. By doing so, we do not change the previous brackets between pairs of moments because the new moments

$$\Delta(AB) := \Delta_1(AB)+\Delta_{AB}C_1 \tag{113}$$

have brackets

$$\begin{aligned}
\{\Delta(A_1B_1),\Delta(A_2B_2)\} \;=\;& \{\Delta_1(A_1B_1),\Delta_1(A_2B_2)\}\\
&-\Delta_{A_1B_1}\{\Delta_1(A_2B_2),C_1\}+\Delta_{A_2B_2}\{\Delta_1(A_1B_1),C_1\}\\
&+\left(\{\Delta_1(A_1B_1),\Delta_{A_2B_2}\}+\{\Delta_{A_1B_1},\Delta_1(A_2B_2)\}+\{\Delta_{A_1B_1},C_1\}\Delta_{A_2B_2}\right.\\
&\left.+\{C_1,\Delta_{A_2B_2}\}\Delta_{A_1B_1}+\{\Delta_{A_1B_1},\Delta_{A_2B_2}\}C_1\right)C_1\\
=\;& \{\Delta_1(A_1B_1),\Delta_1(A_2B_2)\}+O(\Delta^2)+O(C_1)\,.
\end{aligned} \tag{114}$$

However, brackets between expectation values and moments do change according to

$$\begin{aligned}
&\{A+\Delta_AC_1,\Delta_1(A_1B_1)+\Delta_{A_1B_1}C_1\}\\
=\;& \{A,\Delta_1(A_1B_1)\}+\Delta_{A_1B_1}\{A,C_1\}-\Delta_A\{\Delta_1(A_1B_1),C_1\}\\
&+\left(\{A,\Delta_{A_1B_1}\}+\{\Delta_A,\Delta_1(A_1B_1)\}+\{\Delta_A,C_1\}\Delta_{A_1B_1}\right.\\
&\left.+\{C_1,\Delta_{A_1B_1}\}\Delta_A+\{\Delta_A,\Delta_{A_1B_1}\}C_1\right)C_1\\
=\;& \{A,\Delta_1(A_1B_1)\}+\Delta_{A_1B_1}\{A,C_1\}+O(\Delta^2)+O(C_1)
\end{aligned} \tag{115}$$

We can exploit this freedom in order to ensure that all Poisson brackets between $\mathcal{V}$ or $\mathcal{H}$ and any moment including $\mathcal{V}$ or $\mathcal{H}$ vanish:

$$\Delta_{\mathcal{V}^2} \;=\; 0 \tag{116}$$

$$\Delta_{\mathcal{V}\mathcal{H}} \;=\; -\frac{1}{2p_\phi}\Delta(V\phi)+\frac{\mathcal{V}^2\mathcal{H}}{2p_\phi^2}\Delta(\phi^2) \tag{117}$$

$$\Delta_{\mathcal{H}^2} \;=\; -\frac{1}{p_\phi}\Delta(H\phi)-\frac{1}{\mathcal{V}}\Delta(\phi^2)\,. \tag{118}$$

Note the non-trivial nature of this result: The choice of a single Δ_{AB} has to make sure that two relations, $\{\mathcal{V},\Delta(AB)\}=0$ and $\{\mathcal{H},\Delta(AB)\}=0$ are satisfied.

A closer look at brackets of $\mathcal{V}$ and $\mathcal{H}$ with moments including p_ϕ shows that they cannot be made equal to zero by adding terms proportional to C_1. For instance, (107) depends on $\Delta(\mathcal{V}\mathcal{H})$ while (108) depends on $\Delta(\mathcal{V}p_\phi)$. Here, we have to apply our second lesson: After partially solving the constraints, p_ϕ is no longer independent of $\mathcal{V}$ and $\mathcal{H}$. Moreover, while a kinematical product, such as $\widehat{\Delta V}\widehat{\Delta p_\phi}$, is by definition Weyl-ordered, this need not be the case on the physical Hilbert space (which is relevant for partially invariant moments) if the dependence of p_ϕ on $\mathcal{H}$ is taken into account.

We can compute the expected brackets in the following way,

$$\begin{aligned}
\{\mathcal{V},\Delta(\mathcal{V}p_\phi)\} \;=\;& \frac{\langle[\hat{V},(\widehat{\Delta V}\widehat{\Delta p_\phi})_{\rm Weyl}]\rangle}{i\hbar}=\frac{\langle\widehat{\Delta V}[\hat{V},\hat{p}_\phi]+[\hat{V},\hat{p}_\phi]\widehat{\Delta V}\rangle}{2i\hbar}\\
=\;& -\frac{1}{2}\left\langle\widehat{\Delta V}\frac{\widehat{\partial p_\phi}}{\partial H}+\frac{\widehat{\partial p_\phi}}{\partial H}\widehat{\Delta V}\right\rangle\\
=\;& -\frac{1}{2}\left\langle\frac{1}{p_\phi}\left(\widehat{\Delta V}(\widehat{\Delta V}+V)^2(\widehat{\Delta H}+H)(1-\widehat{\Delta p_\phi})\right.\right.\\
&\left.\left.+(\widehat{\Delta V}+V)^2(\widehat{\Delta H}+H)(1-\widehat{\Delta p_\phi})\widehat{\Delta V}\right)\right\rangle\\
=\;& -\frac{1}{2}\left\langle\frac{4VH}{p_\phi}\widehat{\Delta V}^2+\frac{V^2}{p_\phi}\left(\widehat{\Delta V}\widehat{\Delta H}+\widehat{\Delta H}\widehat{\Delta V}\right)-\frac{V^2H}{p_\phi^2}\left(\widehat{\Delta V}\widehat{\Delta p_\phi}+\widehat{\Delta p_\phi}\widehat{\Delta V}\right)\right\rangle\\
&+O(\Delta^2)\\
=\;& -\frac{2\mathcal{V}\mathcal{H}}{p_\phi}\Delta(\mathcal{V}^2)-\frac{\mathcal{V}^2}{p_\phi}\Delta(\mathcal{V}\mathcal{H})+\frac{\mathcal{V}^2\mathcal{H}}{p_\phi^2}\Delta(\mathcal{V}p_\phi)+O(\Delta^2)\,,
\end{aligned} \tag{119}$$

using operators on a physical Hilbert space obtained after deparameterizing by ϕ. Similarly, we expect

$$\{\mathcal{H},\Delta(\mathcal{V}p_\phi)\} = -\frac{p_\phi}{\mathcal{V}^2}\Delta(\mathcal{V}^2)+\frac{1}{2}\Delta(\mathcal{V}p_\phi)\,. \tag{120}$$

It is now possible to bring the brackets (107) and (108) to the form (119) and (120), respectively, by using a redefinition of $\Delta_1(\mathcal{V}p_\phi)$ with

$$\Delta_{\mathcal{V}p_\phi} = -\frac{1}{2p_\phi}\Delta(\mathcal{V}^2)+\frac{\mathcal{V}}{2p_\phi^2}\Delta(\mathcal{V}p_\phi)\,. \tag{121}$$

Similarly,

$$\begin{aligned}\Delta_{\mathcal{H}p_\phi} &= -\frac{1}{2p_\phi}\Delta(\mathcal{V}\mathcal{H})-\frac{1}{2p_\phi}\Delta(\phi p_\phi) \qquad (122)\\ &\quad +\frac{\mathcal{V}}{2p_\phi^2}\Delta(\mathcal{H}p_\phi)\\ \Delta_{p_\phi^2} &= -\frac{1}{p_\phi}\Delta(\mathcal{V}p_\phi)+\frac{\mathcal{V}}{p_\phi^2}\Delta(p_\phi^2) \qquad (123)\end{aligned}$$

yield the expected brackets with $\Delta(\mathcal{H}p_\phi)$ and $\Delta(p_\phi^2)$, respectively:

$$\begin{aligned}\{\mathcal{V},\Delta(\mathcal{H}p_\phi)\} &= -2\frac{\mathcal{V}\mathcal{H}}{p_\phi}\Delta(\mathcal{V}\mathcal{H})-\frac{\mathcal{V}^2}{p_\phi}\Delta(\mathcal{H}^2) \qquad (124)\\ &\quad +\frac{\mathcal{V}\mathcal{H}}{p_\phi^2}\Delta(\mathcal{H}p_\phi)\\ \{\mathcal{H},\Delta(\mathcal{H}p_\phi)\} &= \frac{1}{\mathcal{V}}\Delta(\mathcal{H}p_\phi)-\frac{p_\phi}{\mathcal{V}^2}\Delta(\mathcal{V}\mathcal{H}) \qquad (125)\\ \{\mathcal{V},\Delta(p_\phi^2)\} &= -2\frac{\mathcal{V}^2}{p_\phi}\Delta(\mathcal{H}p_\phi)+2\frac{\mathcal{V}^2\mathcal{H}}{p_\phi^2}\Delta(p_\phi^2) \qquad (126)\\ &\quad -4\frac{\mathcal{V}\mathcal{H}}{p_\phi}\Delta(\mathcal{V}p_\phi)\\ \{\mathcal{H},\Delta(p_\phi^2)\} &= -2\frac{p_\phi}{\mathcal{V}^2}\Delta(\mathcal{V}p_\phi)+\frac{2}{\mathcal{V}}\Delta(p_\phi^2)\,. \qquad (127)\end{aligned}$$

Finally,

$$\Delta_{\mathcal{V}\Lambda}=0 \quad \text{and} \quad \Delta_{\mathcal{H}\Lambda}=-\frac{1}{2p_\phi}\Delta(\phi\Lambda) \tag{128}$$

imply

$$\begin{aligned}\{\mathcal{V},\Delta(\mathcal{V}\Lambda)\} &= \{\mathcal{H},\Delta(\mathcal{V}\Lambda)\} \qquad (129)\\ &= \{\mathcal{V},\Delta(\mathcal{H}\Lambda)\}=\{\mathcal{H},\Delta(\mathcal{H}\Lambda)\}=0\,.\end{aligned}$$

As a consistency check, we can express $\Delta(\mathcal{V}p_\phi)$ as a combination of other moments, solving $C_V=0$, and compare the resulting Poisson bracket $\{\mathcal{V},\Delta(\mathcal{V}p_\phi)\}$ with (119). First, rewriting C_V in terms of partially invariant expectation values and moments results in

$$\begin{aligned}C_V &= -\left(\mathcal{H}^2+\frac{p_\phi^2}{\mathcal{V}^2}-\Lambda\right)\Delta(\mathcal{V}^2)-2\mathcal{V}\mathcal{H}\Delta(\mathcal{V}\mathcal{H})\\ &\quad +2\frac{p_\phi}{\mathcal{V}}\Delta(\mathcal{V}p_\phi)+\mathcal{V}\Delta(\mathcal{V}\Lambda) \qquad (130)\end{aligned}$$

(up to a term proportional to C_ϕ), from which only the imaginary term of the original expression has disappeared. Solving $C_V=0$ and using C_1, we therefore have

$$\Delta(\mathcal{V}p_\phi)=\frac{p_\phi}{\mathcal{V}}\Delta(\mathcal{V}^2)+\frac{\mathcal{V}^2\mathcal{H}}{p_\phi}\Delta(\mathcal{V}\mathcal{H})-\frac{\mathcal{V}^2}{2p_\phi}\Delta(\mathcal{V}\Lambda)\,. \tag{131}$$

Computing $\{\mathcal{V},\Delta(\mathcal{V}p_\phi)\}$ with this expression, taking into account the dependence of p_ϕ on $\mathcal{H}$, indeed results in (119) (up to a term proportional to C_V).

3. *Reduced constraint*

The remaining constraint C_1 written in terms of invariant expectation values and moments is

$$\begin{aligned}\mathcal{C}_\phi &= -\mathcal{V}_1\mathcal{H}_1^2+\frac{p_\phi^2}{\mathcal{V}_1}+\mathcal{V}_1\Lambda-\mathcal{V}_1\Delta_1(\mathcal{H}^2)-2\mathcal{H}_1\Delta_1(\mathcal{V}\mathcal{H})\\ &\quad +\frac{p_\phi^2}{\mathcal{V}_1^3}\Delta_1(\mathcal{V}^2)+\frac{1}{\mathcal{V}_1}\Delta(p_\phi^2)-2\frac{p_\phi}{\mathcal{V}_1^2}\Delta_1(\mathcal{V}p_\phi)\\ &\quad +\Delta_1(\mathcal{V}\Lambda)+i\hbar\mathcal{H}_1\,. \qquad (132)\end{aligned}$$

The moment corrections are of the same form that C_1 has in terms of the kinematical expectation values and moments. This property remains true after a transformation to invariant moments with standard Poisson brackets,

$$\begin{aligned}\mathcal{C}_\phi &= -\mathcal{V}\mathcal{H}^2+\frac{p_\phi^2}{\mathcal{V}}+\mathcal{V}\Lambda-\mathcal{V}\Delta(\mathcal{H}^2)-2\mathcal{H}\Delta(\mathcal{V}\mathcal{H})+\frac{p_\phi^2}{\mathcal{V}^3}\Delta(\mathcal{V}^2)+\frac{1}{\mathcal{V}}\Delta(p_\phi^2)-2\frac{p_\phi}{\mathcal{V}^2}\Delta(\mathcal{V}p_\phi)+\Delta(\mathcal{V}\Lambda)+i\hbar\mathcal{H} \qquad (133)\\ &\quad +\left(-\mathcal{V}\mathcal{H}^2+\frac{p_\phi^2}{\mathcal{V}}+\mathcal{V}\Lambda\right)\left(-2\frac{p_\phi^2}{\mathcal{V}^2}\Delta_{\mathcal{V}}-(2\mathcal{V}\mathcal{H}-i\hbar)\,\Delta_{\mathcal{H}}-\mathcal{V}\Delta_{\mathcal{H}^2}-2\mathcal{H}\Delta_{\mathcal{V}\mathcal{H}}+\frac{p_\phi^2}{\mathcal{V}^3}\Delta_{\mathcal{V}^2}-2\frac{p_\phi}{\mathcal{V}^2}\Delta_{\mathcal{V}p_\phi}+\Delta_{\mathcal{V}\Lambda}\right)\end{aligned}$$

$$\approx -\mathcal{V}\mathcal{H}^2+\frac{p_\phi^2}{\mathcal{V}}+\mathcal{V}\Lambda-\mathcal{V}\Delta(\mathcal{H}^2)-2\mathcal{H}\Delta(\mathcal{V}\mathcal{H})+\frac{p_\phi^2}{\mathcal{V}^3}\Delta(\mathcal{V}^2)+\frac{1}{\mathcal{V}}\Delta(p_\phi^2)-2\frac{p_\phi}{\mathcal{V}^2}\Delta(\mathcal{V}p_\phi)+\Delta(\mathcal{V}\Lambda)+i\hbar\mathcal{H}+O(\Delta^2)\,.$$

However, some of the Poisson brackets of partially invariant moments are different from the kinematical ones (such as $\{\mathcal{V},\Delta(\mathcal{V}p_\phi)\}\neq 0$), which affects the dynamics of expectation values and moments. We can make this explicit by eliminating the p_ϕ-moments using (131) and a similar relation obtained for $\Delta(p_\phi^2)$:

$$\begin{aligned}\mathcal{C}_\phi &= -\mathcal{V}\mathcal{H}^2+\frac{p_\phi^2}{\mathcal{V}}+\mathcal{V}\Lambda-\frac{\Lambda\mathcal{V}^3}{p_\phi^2}\Delta(\mathcal{H}^2)-2\mathcal{H}\Delta(\mathcal{V}\mathcal{H})\\ &\quad+\Delta(\mathcal{V}\Lambda)-\frac{\mathcal{V}^3\mathcal{H}}{p_\phi^2}\Delta(\mathcal{H}\Lambda)+\frac{\mathcal{V}^3}{4p_\phi^2}\Delta(\Lambda^2)+i\hbar\mathcal{H}\end{aligned} \qquad (134)$$

All moments in this expression have standard Poisson brackets. This final expression is (almost) the same as $2p_\phi$ times the generator (64) in the model deparameterized by ϕ, using $p_\phi=-\mathcal{V}\sqrt{\mathcal{H}^2-\Lambda}$. The only difference is the imaginary contribution to (134), to which we turn now.

The transformation to partially invariant moments has led to an imaginary part $\hbar\mathcal{H}$ which indicates that the Weyl-ordered operator used for C_1 was not a suitable ordering. In order to understand this term, we first derive and look at a different version of the reduced constraint obtained after choosing T as internal time, that is, using combinations of T-moments instead of ϕ-moments to construct partial invariants. Although we have not explicitly performed deparameterization, we have implicitly chosen an internal time by deciding to express partially reduced expectation values and moments in terms of ϕ-moments: In the gauge that leads to ϕ as internal time, all partially reduced moments equal their kinematical versions. In a gauge that leads to T as internal time, however, the partially invariant moments differ from their kinematical versions. We have already noted that these expressions are useful because they tell us how we should compare moments obtained with different choices of internal time: We should not directly compare V in the two versions with ϕ and T, respectively, as internal time, but rather V in the ϕ-gauge with $\mathcal{V}$ in the T-gauge.

We could have decided to express partially reduced expectation values and moments such that they equal their kinematical versions in the gauge that leads to T as internal time. The resulting expressions,

$$\mathcal{W}_1 = V-\frac{2H}{V}\Delta(VT)-2\Delta(HT)+2\frac{\Lambda}{V}\Delta(T^2) \qquad (135)$$

$$\mathcal{K}_1 = H+4\frac{H}{V}\Delta(HT)+4\frac{Hp_\phi^2}{V^4}\Delta(T^2)-\frac{2}{V}\left(\Delta(T\Lambda)+\frac{1}{2}i\hbar\right) \qquad (136)$$

$$\Delta_1(\mathcal{W}^2) = \Delta(V^2)-4H\Delta(VT)+4H^2\Delta(T^2) \qquad (137)$$

$$\Delta_1(\mathcal{W}\mathcal{K}) = \Delta(VH)+2\frac{p_\phi^2}{V^3}\Delta(VT)-2H\Delta(HT)-4\frac{Hp_\phi^2}{V^3}\Delta(T^2) \qquad (138)$$

$$\Delta_1(\mathcal{K}^2) = \Delta(H^2)+4\frac{p_\phi^2}{V^3}\Delta(HT)+4\frac{p_\phi^4}{V^6}\Delta(T^2) \qquad (139)$$

$$\Delta_1(\mathcal{W}p_\phi) = \Delta(Vp_\phi)-2H\Delta(p_\phi T) \qquad (140)$$

$$\Delta_1(\mathcal{W}\Lambda) = \Delta(V\Lambda)-2H\Delta(T\Lambda) \qquad (141)$$

$$\Delta_1(\mathcal{K}\Lambda) = \Delta(H\Lambda)+2\frac{p_\phi^2}{V^3}\Delta(T\Lambda)\,, \qquad (142)$$

differ from the previous expressions. This fact is not surprising because they correspond to two different Dirac observables, $\hat{V}(\phi)$ and $\hat{H}(\phi)$ for $\mathcal{V}$ and $\mathcal{H}$, and $\hat{V}(T)$ and $\hat{H}(T)$ for $\mathcal{W}$ and $\mathcal{K}$. However, we have to revisit the question of how a choice of internal time, even an implicit one, affects the dynamics, and therefore covariance.

For our new set of variables, we compute the effective constraint

$$\begin{aligned}\mathcal{C}_T &= -\mathcal{W}_1\mathcal{K}_1^2+\frac{p_\phi^2}{\mathcal{W}_1}+\mathcal{W}_1\Lambda-\mathcal{W}_1\Delta_1(\mathcal{K}^2)-2\mathcal{K}_1\Delta_1(\mathcal{W}\mathcal{K})+\frac{p_\phi^2}{\mathcal{W}_1^3}\Delta_1(\mathcal{W}^2)+\frac{1}{\mathcal{W}_1}\Delta(p_\phi^2)-2\frac{p_\phi}{\mathcal{W}_1^2}\Delta_1(\mathcal{W}p_\phi)+\Delta_1(\mathcal{W}\Lambda)\\ &\quad -i\hbar\mathcal{K}_1\end{aligned} \qquad (143)$$

$$\begin{aligned}&\approx -\mathcal{W}\mathcal{K}^2+\frac{p_\phi^2}{\mathcal{W}}+\mathcal{W}\Lambda-\mathcal{W}\Delta(\mathcal{K}^2)-2\mathcal{K}\Delta(\mathcal{W}\mathcal{K})+\frac{p_\phi^2}{\mathcal{W}^3}\Delta(\mathcal{W}^2)+\frac{1}{\mathcal{W}}\Delta(p_\phi^2)-2\frac{p_\phi}{\mathcal{W}^2}\Delta(\mathcal{W}p_\phi)+\Delta(\mathcal{W}\Lambda)\\ &\quad -i\hbar\mathcal{K}+O(\Delta^2)\,.\end{aligned} \qquad (144)$$

We eliminate $\Delta(\mathcal{W}\Lambda)$ by solving $C_V=0$, leaving only moments with standard Poisson brackets in

$$\mathcal{C}_T = -\mathcal{W}\mathcal{K}^2+\frac{p_\phi^2}{\mathcal{W}}+\mathcal{W}\Lambda-\mathcal{W}\Delta(\mathcal{K}^2)+\frac{3p_\phi^2}{\mathcal{W}^3}\Delta(\mathcal{W}^2)$$

$$+\frac{1}{\mathcal{W}}\Delta(p_\phi^2)-\frac{4p_\phi}{\mathcal{W}^2}\Delta(\mathcal{W}p_\phi)-i\hbar\mathcal{K}\,. \tag{145}$$

There is again an imaginary sign, but it has the opposite sign compared with the constraint obtained after choosing ϕ as internal time. It is therefore impossible to remove the term with a single reordering of the kinematical constraint operator. Just as before in deparameterized models, we have to discuss the question of ordering choices.

It is easier to understand this issue for $\mathcal{C}_T$ because the Λ-dependent term in the constraint is polynomial in canonical variables, unlike the p_ϕ-dependent term. The imaginary term in the reduced constraints can be traced back to the complex value assigned to $\Delta(V\Lambda)$ after solving the constraint $C_V=0$. While $\hat{V}$ and $\hat{\Lambda}$ commute on a kinematical Hilbert space, this is not the case on the physical Hilbert space where solving the constraint implies that we have a quantized version of the classical on-shell relationship $\Lambda=H^2-p_\phi^2/V^2$. If we assume that this expression, which does not give rise to ordering choices between $\hat{H}$ and $\hat{V}$ or $\hat{V}$ and $\hat{p}_\phi$, is simply quantized to $\hat{\Lambda}=\hat{H}^2-\hat{p}_\phi^2\hat{V}^{-2}$ on a physical Hilbert space, we have the non-zero commutator $[\hat{\Lambda},\hat{V}]=2i\hbar\hat{H}$. The result $\mathcal{C}_T$ can be interpreted as describing a constraint in which $i\hbar\hat{H}$ has been subtracted from the original constraint operator $\hat{C}$, which we assumed to be Weyl-ordered. The ordering of the Λ-dependent term is then

$$\frac{1}{2}(\hat{V}\hat{\Lambda}+\hat{\Lambda}\hat{V})-i\hbar\hat{H}=\frac{1}{2}(\hat{V}\hat{\Lambda}+\hat{\Lambda}\hat{V})-\frac{1}{2}[\hat{\Lambda},\hat{V}]=\hat{V}\hat{\Lambda}\,. \tag{146}$$

This ordering is consistent with the generator (66) obtained in the deparameterized model, where multiplication with $\hat{V}^{-1}$ from the left solves the constraint for Λ if $\hat{V}$ is ordered to the left of Λ.

We can see the same behavior in the imaginary contribution to $\mathcal{C}_\phi$ obtained with ϕ as internal time, although ordering questions of the non-polynomial term p_ϕ^2/V are more involved. After solving the constraint, we expect the relationship $p_\phi^2=V^2H^2-\Lambda V^2$, which is polynomial in canonical variables. Without taking a square root, we assume totally symmetric ordering of this expression, which is

$$\begin{aligned}\hat{p}_\phi^2 &= \frac{1}{6}\left(\hat{V}^2\hat{H}^2+\hat{V}\hat{H}\hat{V}\hat{H}+\hat{V}\hat{H}^2\hat{V}+\hat{H}\hat{V}^2\hat{H}+\hat{H}\hat{V}\hat{H}\hat{V}+\hat{H}^2\hat{V}^2\right)-\Lambda\hat{V}^2\\ &= \hat{V}\hat{H}^2\hat{V}-3\hbar^2-\Lambda\hat{V}^2\,.\end{aligned} \tag{147}$$

The commutator with $\hat{V}$ is therefore

$$[\hat{p}_\phi^2,\hat{V}]=2i\hbar\hat{V}\hat{H}\hat{V}\,. \tag{148}$$

For a symmetric ordering of $\hat{V}^{-1}$ and $\hat{p}_\phi^2$ in the constraint operator, adding $i\hbar\hat{H}$ as indicated by $\mathcal{C}_\phi$ implies that the relevant ordering is

$$\frac{1}{2}\left(\hat{V}^{-1}\hat{p}_\phi^2+\hat{p}_\phi^2\hat{V}^{-1}\right)+i\hbar\hat{H}=\frac{1}{2}\left(\hat{V}^{-1}\hat{p}_\phi^2+\hat{p}_\phi^2\hat{V}^{-1}\right)+\frac{1}{2}\hat{V}^{-1}[\hat{p}_\phi^2,\hat{V}]\hat{V}^{-1}=\hat{V}^{-1}\hat{p}_\phi^2\,, \tag{149}$$

which is consistent with the ordering required by the generator (60) in the model deparameterized by ϕ.

In this way, we are able to interpret the imaginary contributions. However, it is impossible to formulate these orderings at the level of the kinematical constraints because $\hat{V}$, $\hat{\Lambda}$ and $\hat{p}_\phi$ commute on the kinematical Hilbert space. Instead, it is possible to change the ordering of the term $-VH^2$ in the kinematical constraint in order to obtain the same imaginary contributions as indicated after solving the constraints. Equation (67) shows that the negative imaginary term, obtained for T as internal time, can be obtained if we choose the ordering $(\hat{V}\hat{H}^2)'=\hat{V}\hat{H}^2$ in the kinematical constraint operator instead of totally symmetric ordering. The constraint operator $\hat{C}'=\hat{C}_{\rm Weyl}+i\hbar\hat{H}$ then implies a real constraint $\mathcal{C}'_T=\mathcal{C}_T+i\hbar\mathcal{K}$, or

$$\begin{aligned}\mathcal{C}'_T &= -\mathcal{W}\mathcal{K}^2+\frac{p_\phi^2}{\mathcal{W}}+\mathcal{W}\Lambda-\mathcal{W}\Delta(\mathcal{K}^2)+\frac{3p_\phi^2}{\mathcal{W}^3}\Delta(\mathcal{W}^2)\\ &\quad+\frac{1}{\mathcal{W}}\Delta(p_\phi^2)-\frac{4p_\phi}{\mathcal{W}^2}\Delta(\mathcal{W}p_\phi)\,.\end{aligned} \tag{150}$$

Similarly, we have

$$\hat{H}^2\hat{V} = \frac{1}{3}(\hat{V}\hat{H}^2+\hat{H}\hat{V}\hat{H}+\hat{H}^2\hat{V})+i\hbar\hat{H} = (\hat{V}\hat{H}^2)_{\rm Weyl}+i\hbar\hat{H}\,. \tag{151}$$

If we use the ordering $(\hat{V}\hat{H}^2)'' = \hat{H}^2\hat{V}$ in a reordered constraint operator $\hat{C}''$, we therefore have $\hat{C}'' = \hat{C}_{\rm Weyl} - i\hbar\hat{H}$ and the imaginary parts in $\mathcal{C}''_\phi = \langle\hat{C}''\rangle = \mathcal{C}_\phi - i\hbar\mathcal{H}$ with partially invariant moments corresponding to choosing ϕ as internal time cancel out:

$$\begin{aligned}\mathcal{C}''_\phi \;=\; & -\mathcal{V}\mathcal{H}^2 + \frac{p_\phi^2}{\mathcal{V}} + \mathcal{V}\Lambda - \frac{\Lambda\mathcal{V}^3}{p_\phi^2}\Delta(\mathcal{H}^2) - 2\mathcal{H}\Delta(\mathcal{V}\mathcal{H}) + \Delta(\mathcal{V}\Lambda)\\ & -\frac{\mathcal{V}^3\mathcal{H}}{p_\phi^2}\Delta(\mathcal{H}\Lambda) + \frac{\mathcal{V}^3}{4p_\phi^2}\Delta(\Lambda^2)\,.\end{aligned} \tag{152}$$

Formally, the reduced constraints obtained for T and ϕ as internal time are now identical, up to terms proportional to constrants C_1 and C_f. We will refer to this constraint as $\mathcal{C}^*$, and write the constraint operator as $\hat{C}$ with the understanding that the ordering has been adapted to the choice of how one derives the reduced constraint. Independently of the ordering,

$$\mathcal{C}_* \approx {\rm Re}\,\mathcal{C}_\phi \approx {\rm Re}\,\mathcal{C}_T\,. \tag{153}$$

4. Coordinate time

With a real-valued effective constraint $\mathcal{C}_*$ in terms of partial 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

$$\mathcal{N}\mathcal{C}_* = N_1C_1 + \sum_f N_fC_f = \langle(N_1+N_f(\hat{f}-f))\hat{C}\rangle = \langle\hat{N}\hat{C}\rangle \tag{154}$$

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 can therefore be implemented within the effective constrained system, but it amounts to a gauge choice different from most deparameterized models. If we consider only moment corrections, there are gauge transformations between proper time and all internal times within the effective constrained system. Reparameterization invariance is therefore preserved, including transformations from proper time to internal time and between different internal times. However, no gauge transformation to proper time exists within a deparameterized model (on a fixed physical Hilbert space), in which the gauge fixing can no longer be changed.

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 $\mathcal{N}\mathcal{C}_*$ 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 coordinate time therefore allows the same changes of time coordinates as in the classical theory and is, in this sense, time reparameterization invariant.

V. DISCUSSION

We have pointed out that time reparameterization invariance of effective equations is not automatically 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 and cosmological time, 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. Different factor orderings then merely amount to the usual ordering ambiguities and do not affect covariance.

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, or to derive partial invariants that show how expectation values and moments obtained in different deparameterizations should be compared. 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 cannot be assumed to give correct moment corrections in effective equations, strengthening the results of [13]. Deparameterized formulations of quantum cosmological models with significant quantum fluctuations should, therefore, be interpreted with great care.

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Appendix A: Canonical effective methods: Brief review

Canonical effective methods [26, 27] formulate the usual evolution equations of wave functions (in a Schrödinger picture) or operators (in a Heisenberg picture) in terms of coupled equations for expectation values and moments. Given a set of basic operators such as $\hat{q}$ and $\hat{p}$, there is therefore an extension of the classical phase space, which can be realized with coordinates $q = \langle\hat{q}\rangle$ and $p = \langle\hat{p}\rangle$ for a given state, by infinitely many moments

$$\Delta(q^a p^b) = \langle(\hat{q}-q)^a(\hat{p}-p)^b\rangle_{\rm symm} \qquad \text{(A1)}$$

in totally symmetric (or Weyl) ordering.

The variables define an extended phase space via a Poisson bracket

$$\{A,B\} = \frac{\langle[\hat{A},\hat{B}]\rangle}{i\hbar} \qquad \text{(A2)}$$

defined through the commutator. This equation can be applied directly to the basic expectation values, such that $\{q,p\} = \langle[\hat{q},\hat{p}]\rangle/i\hbar = 1$. In order to apply the Poisson bracket to moments, we use linearity in (A2) and require the Leibniz rule for products of expectation values. For instance, for the second-order moment $\Delta(p^2) = (\Delta p)^2$, we compute

$$\begin{aligned}\{q,\Delta(p^2)\} &= \{\langle\hat{q}\rangle, \langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2\}\\ &= \{\langle\hat{q}\rangle,\langle\hat{p}^2\rangle\} - 2\langle\hat{p}\rangle\{\langle\hat{q}\rangle,\langle\hat{p}\rangle\}\\ &= \frac{\langle[\hat{q},\hat{p}^2]\rangle}{i\hbar} - 2\langle\hat{p}\rangle\frac{\langle[\hat{q},\hat{p}]\rangle}{i\hbar} = 0\,,\end{aligned}$$

applying linearity and the Leibniz rule in the second line, and (A2) in the last line. More generally, the Poisson bracket of a basic expectation value with any moment is zero [26]. (This is one advantage of choosing central, Weyl-ordered moments to parameterize a state.)

Any operator, such as a Hamiltonian $\hat{H}$ or a constraint $\hat{C}$, gives rise to a function of expectation values and moments through the expectation value $\langle\hat{H}\rangle$ or $\langle\hat{C}\rangle$, respectively, taken in the state that belongs to a given set of basic expectation values and moments. In general, it can be difficult to evaluate this function, but if $\hat{H} = H(\hat{q},\hat{p})$, say, is given as a Weyl-ordered function of basic operators, for semiclassical purposes the expansion

$$\langle\hat{H}\rangle = \langle H(q+(\hat{q}-q), p+(\hat{p}-p))\rangle = H(q,p) + \sum_{a+b=2}^{\infty}\frac{1}{a!b!}\frac{\partial^{a+b}H(q,p)}{\partial q^a\partial p^b}\Delta(q^a p^b) \qquad \text{(A3)}$$

is sufficient. Moreover, if $H(\hat{q},\hat{p})$ is a polynomial, the formal expansion (A3) is exact, and merely rearranges the expectation value of a polynomial in basic operators in terms of central moments.

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