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Uniqueness of minimal loop quantum cosmology dynamics

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We show that the Hamiltonian of isotropic loop quantum cosmology is selected by physical criteria plus a choice implementing Occam's razor. We also parametrize the freedom when this choice is relaxed and show boundedness of energy density for a broad class of cases. A criterion used is covariance under dilations, the continuous diffeomorphisms remaining in this context, which are not canonical but conformally canonical transformations. We propose how to implement such transformations in quantum theory. Removal of the infrared regulator makes the result independent of ordering ambiguities.

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I. INTRODUCTION

The epistemic value of "simplicity" in a theory—in the sense of parsimony of postulates—goes beyond aesthetics. Simplicity is central to the effectiveness of the scientific method itself. Given a prediction from a theory, there is the question: If the prediction fails, how should the theory be modified? The more postulates in a theory, the more unmanageable this part of the scientific method becomes. Cast another way: another epistemic value central to science is that a theory make "risky" predictions [1]. The fewer the postulates, the fewer ways there are to modify the theory in the face of a negative result, and hence the greater the risk.

The role of *uniqueness theorems* is to reduce a theory to a minimal set of postulates. With predictions starting to be made in loop quantum cosmology (LQC) [2–5], it is thus important to have uniqueness theorems for LQC. Previous works [6–8] have addressed the uniqueness of the kinematics of LQC. The present work extends those results to include dynamics. Together, these works show that the predominant model of LQC is uniquely determined by basic physical principles, plus only two choices, thus bringing out its simplicity.

A simple formulation of a theory also makes clear to the wider scientific community the assumptions that underlie it. By stripping out the technicalities and revealing the physical content of LQC, the present work makes the theory more compelling to those working outside the field.

Loop quantum cosmology is a quantization of the gravitational degrees of freedom at the cosmological scale using the methods of loop quantum gravity (LQG), an approach to quantum gravity in which Einstein's fundamental principle of *general covariance*—or equivalently, in its active form, *diffeomorphism covariance*—is central. The predominant model for LQC is the so-called "improved dynamics", introduced by Ashtekar, Pawlowski, and Singh (APS) [9]. With the results of this paper, it is established that both the kinematics and dynamics of this model are uniquely selected by the following physical principles:

(i) *(Residual) diffeomorphism covariance* of both the kinematical framework as well as the Hamiltonian operator $\hat{H}$.
(ii) that $\hat{H}$ be *Hermitian*.
(iii) that $\hat{H}$ have the *correct classical limit*.

together with the following two choices:

(1) That the phase space functions with direct quantum analogues be the restrictions of those in LQG. This is the only place where LQG enters into the assumptions. We call this the *loop hypothesis*.
(2) That the number of terms in $\hat{H}$, naturally defined, be *minimal*.

The first of the above two choices, via the kinematical uniqueness theorems [6,7,10], selects a unique kinematical Hilbert space of states, namely that of [11]. In the present work, which focuses on dynamics, the loop hypothesis thus implies that the Hamiltonian must act on this space of states.

Part of what makes the present uniqueness theorem possible is that, in LQC, one must take the limit of a *large volume* of the fiducial cell, which serves as an infrared cutoff [12]. Specifically, the commutators among the basic variables in LQC scale as the inverse of the volume of the fiducial cell [13,14], so that in the limit in which the infrared regulator is removed, *all operator ordering ambiguities* in the definition of $\hat{H}$ disappear. This is what allows the present uniqueness result to be stronger than that in the prior work [14], where only uniqueness up to leading and subleading orders in $\hbar$ was achieved. Similar reasoning was used in [12], where the authors point out that inverse volume corrections to the Hamiltonian do not have any physical meaning because they are cell-dependent and vanish once the regulator is removed.

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A second key element of the present work is a quantum equation expressing covariance of a given operator with respect to residual diffeomorphisms in LQC. These residual diffeomorphisms—dilations—are not canonical but, rather, *conformally canonical* transformations. We introduce a method for implementing such transformations in quantum theory which strictly generalizes the standard way of implementing canonical transformations. The resulting quantum covariance condition is well defined for any operator. This contrasts with the covariance condition introduced in [14], which is more complicated and is well defined only for operators satisfying a certain analyticity assumption, but is otherwise equivalent to the condition defined here.

We furthermore note that the question of uniqueness of dynamics in LQC was first investigated in the work [15], which showed how residual diffeomorphism invariance selected the standard dynamics of LQC [9] from a one-parameter family of possible dynamics. The present work starts from no such restriction.

It is also important to mention that if the single choice being imposed on the dynamics—minimality—is removed, then Hamiltonians other than the standard one also become possible, in particular the "$\bar{\mu}$" versions of the dynamics proposed and investigated in [2,16–21]. The present work gives a compact parametrization of the possible Hamiltonians when minimality is relaxed. We note that even when minimality is relaxed, for any finite number of terms, as defined in this paper, the Big Bang singularity is resolved in the sense that energy density is bounded.

This paper summarizes the results and central argument of a more detailed companion paper to appear soon [10].

II. BACKGROUND

In this section we briefly review the required background material (for more details, see [12,22,23]). In LQG the gravitational phase space variables are given by a SU(2) connection A_a^i and a densitized triad E_i^a. We will consider the simple, $k=0$, spatially homogeneous and isotropic model. Let $\mathring{e}_i^a$ be an arbitrarily chosen flat fiducial triad, and $\mathring{\omega}_a^i$ the corresponding cotriad. Then by fixing the gauge we can write

$$A_a^i = \tilde{c}\mathring{\omega}_a^i, \qquad E_i^a = \tilde{p}\mathring{e}_i^a. \tag{1}$$

Thus, the phase space is two-dimensional and parametrized by $(\tilde{c},\tilde{p})$. Because the fields are homogeneous on a noncompact slice, the integral defining the symplectic structure, and hence Poisson brackets, requires introducing an infrared regulator. A choice of compact region $\mathcal{V}$, the "fiducial cell", provides such a regulator, which must be removed before extracting physical results from the theory. Let V_o denote the volume of $\mathcal{V}$ with respect to the metric $\mathring{q}_{ab}$ determined by $\mathring{e}_i^a$. The nonvanishing Poisson brackets are then

$$\{\tilde{c},\tilde{p}\} = \frac{\kappa\gamma}{3V_o}. \tag{2}$$

Upon defining the rescaled variables

$$c \coloneqq V_o^{1/3}\tilde{c}, \qquad p \coloneqq V_o^{2/3}(\det\mathring{q})^{-1/2}\tilde{p},$$

we obtain Poisson brackets independent of V_o,

$$\{c,p\} = \frac{\kappa\gamma}{3},$$

where $\kappa = 8\pi G$ with G the Newton constant and γ is the Barbero-Immirzi parameter. Because of the underlying symmetries only the Hamiltonian constraint remains to be imposed. We choose as our lapse function $N = |p|^{3n/2}$, so that $n=0$ corresponds to the proper time gauge, and $n=1$ corresponds to the harmonic time gauge—both common choices in the literature. The gravitational part of the Hamiltonian constraint is then given by

$$H = \frac{-3}{\kappa\gamma^2}|p|^{\frac{3n+1}{2}}c^2.$$

The group of diffeomorphisms preserving the gauge-fixing (1), and acting nontrivially on (c,p), is generated by parity and the one-parameter family of dilations. Parity is defined by $\Pi_*\mathring{e}_i^a = -\mathring{e}_i^a$ and $\Pi(p_o) = p_o$ with p_o an arbitrary center, with resulting action $(c,p)\mapsto(-c,-p)$. The dilations are diffeomorphisms generated by the "radial" vector field r^a defined by $\partial_b r^a = \delta_b^a$ and $r^a(p_o)=0$, where ∂_a is the covariant derivative determined by $\mathring{q}_{ab}$. The resulting action is

$$(c,p)\mapsto(e^{-t}c, e^{-2t}p), \tag{3}$$

with real parameter t, with H transforming as

$$H(e^{-t}c, e^{-2t}p) = e^{-3(n+1)t}H. \tag{4}$$

Note that the action of dilations here differs from that in [6]: in contrast to that work, the methods developed in this paper do not require dilations to act on the fiducial cell.

The set of phase space functions with direct quantum analogues in LQG is that spanned by fluxes of E_i^a through analytic surfaces, and products of holonomies of A_a^i along analytic paths. When restricted to the above cosmological phase space, this reduces to the span of p, $e^{i\mu c}$ (for $\mu\in\mathbb{R}$), and functions of c vanishing at infinity [24], and generates, in the sense of [25,26], a *quantum algebra* known as the *reduced holonomy-flux algebra* [6]. There is more than one action of residual diffeomorphisms on this algebra consistent with the action (3) on c and p. No matter which action is chosen, *there exists a unique* cyclic representation of the quantum algebra in which the action is unitary, and this representation is *independent* of the action chosen [6,7,10]. The representation so selected acts on the Hilbert space with orthonormal basis $|p\rangle$ for $p \in \mathbb{R}$. The states $|p\rangle$ are then the eigenstates of $\hat{p}$, and the action of $\widehat{e^{i\mu c}}$ on these states is given by $\widehat{e^{i\mu c}}|p\rangle = |p + \frac{\kappa\gamma\hbar}{3}\mu\rangle$. Note that no basic operator corresponding to c exists in the quantum theory—only $e^{i\mu c}$.

We extend the definition of the basic operators to include operators of the form $\widehat{e^{if(p)c}}$, such that they map each momentum eigenstate $|p\rangle$ to $|F(p)\rangle$, where $F(p)$ is the flow, evaluated at unit time, generated by the vector field $\kappa\gamma\hbar f(p)\frac{d}{dp}$. In particular, for $f(p) = \lambda|p|^{-1/2}$ with $\lambda \in \mathbb{R}$, one has the operator $\widehat{e^{i\lambda b}}$, with b and its corresponding conjugate variable v defined as

$$b = |p|^{-1/2}c, \qquad v = \mathrm{sgn}(p)|p|^{3/2}, \qquad \{b, v\} = \frac{1}{2}\kappa\gamma.$$

The action of $\widehat{e^{i\lambda b}}$ on $\hat{v}$ eigenstates is therefore simply $\widehat{e^{i\lambda b}}|v\rangle = |v + \frac{\kappa\gamma\hbar}{2}\lambda\rangle$ [9,23]. Under parity, $\Pi\widehat{e^{i\lambda b}}\Pi = \widehat{e^{-i\lambda b}}$ and $\Pi\hat{v}\Pi = -\hat{v}$. b/γ is the Hubble rate and contains all diffeomorphism-invariant gravitational information.

Note that the limit of removal of the infrared regulator—$V_o \to \infty$ as (A_a^i, E_i^a) and hence $(\tilde{c}, \tilde{p})$ are held constant—is equivalent to $v \to \infty$ with b held constant.

III. SELECTION OF THE QUANTUM HAMILTONIAN CONSTRAINT

A. Residual diffeomorphism covariance and Hermiticity

Classically, the flow of a phase space function F under the canonical transformation generated by the Hamiltonian vector field X_Λ, associated to a phase space function Λ, is given by

$$\dot{F} = \mathcal{L}_{X_\Lambda}F = \{\Lambda, F\}.$$

This has the standard quantization

$$\dot{\hat{F}} = \frac{1}{i\hbar}[\hat{\Lambda}, \hat{F}].$$

Isotropic dilations are not canonical, but they are *conformally* canonical: they are generated by a vector field of the form

$$X = \omega X_\Lambda,$$

whose corresponding flow thus takes the form

$$\dot{F} = \mathcal{L}_X F = \omega\mathcal{L}_{X_\Lambda}F = \omega\{\Lambda, F\}.$$

In the case considered in this paper, Λ turns out to be proportional to c, so that only its exponential has an operator analogue in LQC. This leads us to rewrite the above equation as

$$\dot{F} = \omega\frac{1}{i\lambda}e^{-i\lambda\Lambda}\{e^{i\lambda\Lambda}, F\}. \tag{5}$$

This leads to the quantum equation

$$\dot{\hat{F}} = \hat{\omega} \star \left(\frac{-1}{\lambda\hbar}\widehat{e^{-i\lambda\Lambda}}\left[\widehat{e^{i\lambda\Lambda}}, \hat{F}\right]\right), \tag{6}$$

where $\star$ denotes a choice of ordering for operator products. Note that Eq. (5) is independent of λ; however, the quantization (6) is not. In the case when ω is a constant and one uses the Schrödinger representation, (6) reduces to the standard flow generated by Λ only in the $\lambda \to 0$ limit, and hence we make this choice:

$$\dot{\hat{F}} = \frac{-1}{\hbar}\hat{\omega} \star \lim_{\lambda\to 0}\left(\frac{1}{\lambda}\widehat{e^{-i\lambda\Lambda}}\left[\widehat{e^{i\lambda\Lambda}}, \hat{F}\right]\right). \tag{7}$$

We now use the fact that X is the generator of dilations, so that $\mathcal{L}_X p = -2p$ and $\mathcal{L}_X c = -c$, and $X = \omega(c,p)X_{\Lambda(c,p)}$. Because c has no operator analogue in LQC, we make ω independent of c which, together with the requirement that X_Λ be a generator of canonical transformations, determines ω up to an overall factor M: $\omega = -Mv$. Then Λ is determined up to an additive constant l, $\Lambda = \frac{6}{\kappa\gamma}(M^{-1}b + l)$, and we get

$$X = -MvX_{\frac{6}{\kappa\gamma}(M^{-1}b+l)}.$$

Because of their natural appearance, we will use the variables (b, v) at this point. The Hamiltonian flows under the action of dilations as $\mathcal{L}_X H = -3(n+1)H$, and thus we impose the covariance condition $\dot{\hat{H}} = -3(n+1)\hat{H}$. Equation (7), for $\hat{F} = \hat{H}$, then gives

$$\frac{-M}{\hbar}\hat{v} \star \lim_{\lambda\to 0}\left(\frac{1}{\lambda}\widehat{e^{-i\frac{6\lambda}{\kappa\gamma}(M^{-1}b+l)}}\left[\widehat{e^{i\frac{6\lambda}{\kappa\gamma}(M^{-1}b+l)}}, \hat{H}\right]\right) = 3(n+1)\hat{H}.$$

As expected, l drops out of the equation. Rescaling λ by $\frac{M\kappa\gamma}{6}$ we obtain

$$2\hat{v} \star \lim_{\lambda\to 0}\left(\frac{1}{\lambda}\widehat{e^{-i\lambda b}}\left[\widehat{e^{i\lambda b}}, \hat{H}\right]\right) = -\hbar\kappa\gamma(n+1)\hat{H}. \tag{8}$$

As mentioned above, there is an ordering ambiguity in the product $\star$. For now we choose the Weyl ordering, $\hat{v} \star \hat{O} \coloneqq \frac{1}{2}(\hat{v}\hat{O} + \hat{O}\hat{v})$, and address alternative choices in the next section:

$$-\hbar\kappa\gamma(n+1)\hat{H} = \lim_{\lambda\to 0}(\hat{v}\,\widehat{e^{-i\lambda b}}\,[\widehat{e^{i\lambda b}},\hat{H}] + \widehat{e^{-i\lambda b}}[\widehat{e^{i\lambda b}},\hat{H}]\hat{v}). \tag{9}$$

Equation (9) can be rewritten in terms of the matrix elements of the operator $\hat{H}$ (in the $|v\rangle$ basis),

$$\begin{aligned} &-(n+1)H(v'',v') \\ &\quad = \frac{v'+v''}{2}\lim_{\tilde{\lambda}\to 0}\frac{1}{\tilde{\lambda}}(H(v'',v') - H(v''+\tilde{\lambda},v'+\tilde{\lambda})), \end{aligned}$$

where $\tilde{\lambda} = \frac{\lambda\hbar\kappa\gamma}{2}$. Then, by using the substitution $f_w(u) = H(w+u,u)$, we obtain the differential equation,

$$\frac{w+2u}{2}f'_w(u) = (n+1)f_w(u).$$

The general solution to this equation is

$$H(v'',v') = f_{v''-v'}(v') = B_{v''-v'}(\mathrm{sgn}(v''+v'))\left|\frac{v''+v'}{2}\right|^{n+1} \tag{10}$$

for some functions $B_w(\sigma)$. Using $\widehat{e^{i\frac{2u}{\kappa\gamma\hbar}b}}|v\rangle = |v+u\rangle$, we have

$$\hat{H}|v'\rangle = \sum_{v''}H(v'',v')\widehat{e^{i\frac{2(v''-v')}{\kappa\gamma\hbar}b}}|v'\rangle = \sum_w \widehat{e^{i\frac{2w}{\kappa\gamma\hbar}b}}H(\hat{v}+w,\hat{v})|v'\rangle.$$

Plugging in (10), we can write the operator $\hat{H}$ as

$$\begin{aligned} \hat{H} &= \sum_w \widehat{e^{i\frac{2w}{\kappa\gamma\hbar}b}}\,B_w\left(\mathrm{sgn}\left(\hat{v}+\frac{w}{2}\right)\right)\left|\hat{v}+\frac{w}{2}\right|^{n+1} \\ &= \sum_w \widehat{e^{i\frac{w}{\kappa\gamma\hbar}b}}\,B_w(\mathrm{sgn}(\hat{v}))|\hat{v}|^{n+1}\widehat{e^{i\frac{w}{\kappa\gamma\hbar}b}}. \end{aligned} \tag{11}$$

Next we impose that $\hat{H}$ be Hermitian and parity invariant. These two conditions together force $B_{-w}(\sigma)^* = B_w(\sigma) = B_{-w}(-\sigma)$. This implies

$$B_w(\sigma) = a_{|w|} + i\sigma\mathrm{sgn}(w)b_{|w|}$$

for some $a_{|w|}, b_{|w|}$ real, so that

$$\begin{aligned} \hat{H} &= \sum_w \widehat{e^{i\frac{w}{\kappa\gamma\hbar}b}}(a_{|w|} + i\mathrm{sgn}(w\hat{v})b_{|w|})|\hat{v}|^{n+1}\widehat{e^{i\frac{w}{\kappa\gamma\hbar}b}} \\ &= \sum_{w>0}\widehat{e^{i\frac{w}{\kappa\gamma\hbar}b}}(a_w + i\mathrm{sgn}(\hat{v})b_w)|\hat{v}|^{n+1}\widehat{e^{i\frac{w}{\kappa\gamma\hbar}b}} \\ &\quad + \mathrm{H.c.} + \tilde{a}_0|\hat{v}|^{n+1}, \end{aligned} \tag{12}$$

where H.c. stands for Hermitian conjugate.

Notice that in the Eqs. (11) and (12), the following quantization prescription naturally appears:

$$\widehat{g(v)e^{i\lambda b}} \coloneqq \widehat{e^{i\lambda b/2}}\,\widehat{g(v)}\,\widehat{e^{i\lambda b/2}}. \tag{13}$$

For brevity, we use this prescription to write expressions for $\hat{H}$ in what follows.

We define a "classical analogue" of $\hat{H}$ to be an element of its preimage under a quantization map. The classical analogue of $\hat{H}$ only makes sense if the sum over $w>0$ in (12) contains a countable number of nonzero terms. Let these terms correspond to $w = v_i$ for $i = 1,\ldots,N$ with N possibly infinite. Then we get

$$\hat{H} = \sum_{i=1}^{N}\widehat{(\tilde{a}_i + i\tilde{b}_i\mathrm{sgn}(v))|\hat{v}|^{n+1}e^{i\tilde{A}_i b}} + \mathrm{H.c.} + \tilde{a}_0|\hat{v}|^{n+1}, \tag{14}$$

where $\tilde{a}_0$, $\tilde{a}_i \coloneqq a_{v_i}$, and $\tilde{b}_i \coloneqq b_{v_i}$ are real, and $\tilde{A}_i \coloneqq \frac{2v_i}{\kappa\gamma\hbar} > 0$. Under the quantization prescription (13), the classical analogue of (14) is therefore

$$H = \sum_{i=1}^{N}(\tilde{a}_i + i\tilde{b}_i\mathrm{sgn}(v))|v|^{n+1}e^{i\tilde{A}_i b} + \mathrm{c.c.} + \tilde{a}_0|v|^{n+1}, \tag{15}$$

where c.c. stands for complex conjugate.

We will now go back to using the standard (c,p) variables to facilitate comparison with APS [9]. In these variables we get

$$H = \sum_{i=1}^{N}(\tilde{a}_i + i\tilde{b}_i\mathrm{sgn}(p))|p|^{\frac{3(n+1)}{2}}e^{i\tilde{A}_i\frac{c}{\sqrt{|p|}}} + \mathrm{c.c.} + \tilde{a}_0|p|^{\frac{3(n+1)}{2}}. \tag{16}$$

Note that this H transforms as expected under the action of dilations [see (4)]. We thus conclude that the method used in this paper to impose that $\hat{H}$ be dilation covariant—condition (9)—is in fact equivalent to the method used to impose such covariance in [14], while at the same time eliminating technical assumptions that were needed in [14] and leading to a much simpler argument.

B. Single length scale and correct classical limit

To take the classical limit we let the coefficients $\tilde{a}_0$, $\tilde{a}_i, \tilde{b}_i, \tilde{A}_i$ depend on the classicality parameter $\ell_p \coloneqq \sqrt{\hbar G}$: $\tilde{a}_0(\ell_p), \tilde{a}_i(\ell_p), \tilde{b}_i(\ell_p), \tilde{A}_i(\ell_p)$. We assume now that ℓ_p is the only length scale in the theory. Dimensional arguments easily lead to $\tilde{A}_i(\ell_p) = A_i\ell_p$ and $\tilde{a}_0(\ell_p) = a_0/(G\ell_p^2)$, $\tilde{a}_i(\ell_p) = a_i/(G\ell_p^2), \tilde{b}_i(\ell_p) = b_i/(G\ell_p^2)$. This yields

$$\begin{aligned} \hat{H} = \frac{\ell_p^{-2}}{G}\Bigg(&\sum_{i=1}^{N}\widehat{(a_i + ib_i\mathrm{sgn}(p))|p|^{\frac{3(n+1)}{2}}e^{iA_i\ell_p\frac{c}{\sqrt{|p|}}}} \\ &+ \mathrm{H.c.} + a_0\widehat{|p|^{\frac{3(n+1)}{2}}}\Bigg). \end{aligned} \tag{17}$$

We define the classical limit to be the limit $\ell_p \to 0$, $\hbar \to 0$ of a classical analogue of (17). In this limit classical analogues do not depend on the ordering chosen for the quantization map. Using the ordering (13), one obtains

$$H = \frac{\ell_p^{-2}}{G}\left(\sum_{i=1}^{N}(a_i + ib_i \mathrm{sgn}(p))|p|^{\frac{3(n+1)}{2}} e^{iA_i\ell_p\frac{c}{\sqrt{|p|}}} + \mathrm{c.c.} + a_0|p|^{\frac{3(n+1)}{2}}\right). \tag{18}$$

We expand the exponentials in powers of ℓ_p and match the classical limit to the classical Hamiltonian $H = \frac{-3}{8\pi G\gamma^2}|p|^{\frac{3n+1}{2}}c^2$:

$$\lim_{\ell_p\to 0}\frac{\ell_p^{-2}}{G}|p|^{\frac{3(n+1)}{2}}\left(a_0 + \sum_{i=1}^{N}\left[2a_i - 2b_iA_i\ell_p\mathrm{sgn}(p)\frac{c}{\sqrt{|p|}} - a_iA_i^2\ell_p^2\frac{c^2}{|p|} + \mathcal{O}(\ell_p^3)\right]\right) = \frac{-3}{8\pi G\gamma^2}|p|^{\frac{3n+1}{2}}c^2,$$

giving the following conditions:

$$a_0 + \sum_i 2a_i = 0 \tag{19}$$

$$\sum_i A_i b_i = 0 \tag{20}$$

$$\sum_i A_i^2 a_i = \frac{3}{8\pi\gamma^2}. \tag{21}$$

The class of Hamiltonians (17), (19)–(21), selected *only* by physical criteria and the loop hypothesis, is the first result of this paper. Note, in particular, for $N = 4$, the "$\bar{\mu}$" versions of the Hamiltonians studied in [2,16–21] are included in our framework, while "μ_o" versions of Hamiltonians [27,28] are excluded.

Let us consider a general Hamiltonian $\hat{H}$ in this class. Analysis of various LQC models confirms that the quantum evolution of sharply peaked coherent states is excellently described by an effective Hamiltonian, calculated as the expectation value of the quantum Hamiltonian [9,17,29–32]. In each case, this effective Hamiltonian, on removing the infrared regulator, is exactly equal to the classical analogue in the sense we have defined above. This leads us to use (18) as the effective Hamiltonian H_{grav} for $\hat{H}$. From $H_{\mathrm{grav}} + H_{\mathrm{matt}} = 0$ we get

$$\frac{\ell_p^{-2}}{G}\left(\sum_{i=1}^{N}(a_i + ib_i\mathrm{sgn}(p))|p|^{\frac{3(n+1)}{2}}e^{iA_i\ell_p\frac{c}{\sqrt{|p|}}} + \mathrm{c.c.} + a_0|p|^{\frac{3(n+1)}{2}}\right) = -H_{\mathrm{matt}}.$$

For any minimally coupled matter, H_{matt} is related to the matter energy density ρ by $H_{\mathrm{matt}} = 2N|p|^{\frac{3}{2}}\rho$ with the lapse $N = |p|^{\frac{3n}{2}}$ using our conventions. We obtain

$$\ell_p^{-2}\left(\sum_{i=1}^{N}(a_i + ib_i\mathrm{sgn}(p))e^{iA_i\ell_p\frac{c}{\sqrt{|p|}}} + \mathrm{c.c.} + a_0\right) = -2G\rho.$$

For finite N the left-hand side is manifestly bounded, whence matter density is bounded, so that the Big Bang singularity is resolved in at least this sense. Thus, the present work shows that singularity resolution is achieved in at least one sense for a very broad class of Hamiltonians parametrized above.

C. Minimality

Now we introduce the second key choice: that the number of terms N be the *smallest* such that the Eqs. (19)–(21) are satisfied. This can be viewed as an implementation of Occam's razor. Then $\hat{H}$ is unique up to a single parameter A:

$$\hat{H} = \frac{3}{4\pi A^2 G\gamma^2\ell_p^2}\left(\widehat{|p|^{\frac{3(n+1)}{2}}e^{iA\ell_p\frac{c}{\sqrt{|p|}}}} + \mathrm{H.c.} - 2\widehat{|p|^{\frac{3(n+1)}{2}}}\right).$$

In LQG the area operator has the minimum eigenvalue $\Delta\ell_p^2$ with Δ a dimensionless number. If the parameter A is chosen to be $2\sqrt{\Delta}$ and we choose the lapse with $n = 0$, we obtain *exactly* the "improved dynamics" Hamiltonian introduced in APS [9], including ordering.

IV. ORDERING AMBIGUITY AND THE ROLE OF THE LARGE-VOLUME LIMIT

In the previous sections we assumed a particular ordering prescription for the operator product $\star$ [see (9)]. We will now address this apparent ambiguity by considering alternative choices. Specifically, we demonstrate that in the final quantum theory of cosmology this choice bears no physical significance.

Let us choose an alternative ordering in (8). A general ordering for the operator product $\hat{v} \star \hat{O}$ for $\hat{O}$ arbitrary can be written as

$$\hat{v} \star \hat{O} = \sum_i \alpha_i \hat{v}^{\lambda_i}\hat{O}\hat{v}^{1-\lambda_i}, \tag{22}$$

with coefficients α_i such that $\sum_i \alpha_i = 1$. Then, proceeding as in the previous section, one gets from (8) a differential equation in terms of the matrix elements of the Hamiltonian with alternative ordering $\hat{H}_a$. In the companion paper [10] we give the explicit expressions for the general solution for these matrix elements and show that the operator and its classical analogue take the form

$$\hat{H}_a = \sum_{i=1}^{N}\overline{\tilde{B}_i\left(j\left(\frac{v}{\tilde{A}_i}\right)\right)g\left(\frac{v}{\tilde{A}_i}\right)e^{i\tilde{A}_ib}}, \tag{23}$$

$$H_a = \sum_{i=1}^{N}\tilde{B}_i\left(j\left(\frac{v}{\tilde{A}_i}\right)\right)g\left(\frac{v}{\tilde{A}_i}\right)e^{i\tilde{A}_ib}, \tag{24}$$

where the hat and the classical analogue are again defined as in Eq. (13) and the subsequent text. Here $j\colon \mathbb{R} \to \{0, \ldots, M\}$, $M \in \mathbb{N}$, and $g\colon \mathbb{R} \to \mathbb{R}^+$ are determined by the ordering choice (22), whereas $\tilde{A}_i \in \mathbb{R}$ and $\tilde{B}_i\colon\{0, \ldots, M\} \to \mathbb{R}$, $N \in \mathbb{N} \sqcup \{\infty\}$ are free integration constants.

Recall that v is the physical volume of the fiducial cell which serves as the infrared regulator. This regulator does not have any physical significance: it has been introduced only to provide a well-defined symplectic structure for quantization and has to be removed—that is, the limit $v \to \pm\infty$ taken—as a final and necessary step in defining the quantum theory. In this limit, holding the Hubble rate b/γ constant, the classical analogue (23) turns out to have the asymptotic form $H_a \sim \sum_{i=1}^{N} B_i(\pm)|v|^{n+1} e^{i\tilde{A}_i b}$, which, upon imposing that $\hat{H}_a$ be Hermitian and parity invariant, yields the same classical analogue (15), and therefore the same effective dynamics.

We can also ask whether the *exact quantum* Hamiltonians are equivalent in this same limit, in the sense that

$$\lim_{(|v''|,|v'|)\to(\infty,\infty)} \frac{H_a(v'', v') + C}{H(v'', v') + C} = 1, \qquad (25)$$

where C is any nonzero constant introduced to avoid division by zero. Also this much stronger condition is true, as long as the number of terms in (23) is *finite*. For the technical details of these arguments, we refer the reader to the companion paper.

In this paper we have shown how the dynamics of LQC are uniquely selected by standard physical criteria plus minimality. We have parametrized the possible dynamics when minimality is relaxed, and have shown singularity resolution, in the sense of boundedness of energy density, as long as the number of terms is finite.

A crucial physical criterion imposed is covariance of the Hamiltonian operator under residual diffeomorphisms. A definition of the action of such diffeomorphisms as a flow in the space of operators has been introduced in this paper and makes the strong uniqueness result possible. This definition arises as an application of a more general solution to the problem of implementing noncanonical transformations in quantum theory which we have also here proposed, with potentially broad applicability outside quantum gravity. Any approach to quantum cosmology, whether loop or not, must grapple with this problem in view of the symmetries of general relativity and must use a solution such as the one in the present work.

This solution provides a useful tool for future investigations in quantum cosmology. In full quantum gravity, all states are invariant under all diffeomorphisms, including dilations; that states in quantum cosmology are not is an artifact of the infrared regulator. The implementation of dilations in this paper opens the interesting possibility of considering *mixed states*, that is, density matrices, in quantum cosmology, which are invariant under dilations as well. In LQC specifically, this tool can also be used to improve the kinematical uniqueness results in [6] as we show in the companion paper [10]. In particular, such an improvement dispenses with the need to define dilations as acting on the fiducial cell.

In the parallel work [10] we have also extended this result by including matter degrees of freedom, in particular the free massless scalar field commonly used in LQC. Using new results by Fleischhack [33], this work first establishes *kinematical* uniqueness which selects the polymer quantization for the scalar field [34,35]. The same criteria used in the foregoing sections of this paper then lead to a unique matter part of the Hamiltonian operator [10]. For the lapse equal to 1, in the limit of removal of the infrared regulator, the matrix elements of this uniquely selected Hamiltonian are asymptotic, and therefore equivalent, to those in Sec. II of [34], hence, by the argument in this same reference, equivalent to those of the usual matter Hamiltonian used in the LQC literature.

Extensions to other spatially flat homogeneous loop quantum cosmologies are also possible. In particular, for Bianchi I, we obtain results [10] similar to those in [14], but now with the exact uniqueness made possible by the removal of the infrared regulator considered in this paper.

The fact that physical principles, together with the loop hypothesis and minimality, are sufficient to uniquely determine the dynamics is remarkable. However, this means that the resulting dynamics knows *nothing about any particular choice of dynamics for full loop quantum gravity*. To allow for information about such a choice, it seems that one must relax the minimality assumption. If one does this, the family of Hamiltonians (17), (19)–(21) selected in this paper becomes a potentially powerful tool for determining which LQC dynamics correspond to a given full theory dynamics: By truncating the sum at some finite N, the family has only a finite number of parameters, which then can be fixed by comparing a finite number of calculations in LQC with the corresponding calculations in the full theory using the dynamics of interest. In particular, such a method for determining the LQC dynamics guarantees that the result will be of the "$\bar{\mu}$" type known to be required for results consistent with known physics [9].

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