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Loop quantum cosmology of Bianchi type I models

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The ''improved dynamics'' of loop quantum cosmology is extended to include anisotropies of the Bianchi type I model. As in the isotropic case, a massless scalar field serves as a relational time parameter. However, the extension is nontrivial because one has to face several conceptual subtleties as well as technical difficulties. These include a better understanding of the relation between loop quantum gravity and loop quantum cosmology, handling novel features associated with the nonlocal field strength operator in presence of anisotropies, and finding dynamical variables that make the action of the Hamiltonian constraint manageable. Our analysis provides a conceptually complete description that overcomes limitations of earlier works. We again find that the big-bang singularity is resolved by quantum geometry effects but, because of the presence of Weyl curvature, Planck scale physics is now much richer than in the isotropic case. Since the Bianchi I models play a key role in the Belinskii, Khalatnikov, Lifshitz conjecture on the nature of generic spacelike singularities in general relativity, the quantum dynamics of Bianchi I cosmologies is likely to provide considerable intuition about the fate of generic spacelike singularities in quantum gravity. Finally, we show that the quantum dynamics of Bianchi I cosmologies projects down *exactly* to that of the Friedmann model. This opens a new avenue to relate more complicated models to simpler ones, thereby providing a new tool to relate the quantum dynamics of loop quantum gravity to that of loop quantum cosmology.

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I. INTRODUCTION

Loop quantum gravity (LQG) [1–3] is a nonperturbative, background independent approach to the unification of general relativity and quantum physics. One of its key features is that space-time geometry is treated quantum mechanically from the beginning. Loop quantum cosmology (LQC) [4,5] is constructed by applying methods of LQG to minisuperspaces obtained by a symmetry reduction of general relativity. In the homogeneous, isotropic cosmological models with a massless scalar field, quantum geometry effects of LQG have been shown to create a new repulsive force in the Planck regime. The force is so strong that the big bang is replaced by a specific type of quantum bounce. In the $k = 0$, $\Lambda = 0$ case, the force rises very quickly once the scalar curvature reaches $\sim -0.15\pi/\ell_{\rm Pl}^2$ (or matter density ρ reaches $\sim 0.01\rho_{\rm Pl}$) to cause the bounce but also dies very quickly after the bounce once the scalar curvature and the density fall below these values. Therefore outside the Planck regime the quantum space-time of LQC is very well approximated by the space-time continuum of general relativity. This scenario is borne out in the $k = 0$, $\Lambda = 0$ models [6–13], $\Lambda \neq 0$ models [14,15], the $k = 1$ closed model [16,17], the $k = -1$ open model [18], and the $k = 0$ model with an inflationary potential with phenomenologically viable parameters [19]. Going beyond the big-bang and big-crunch singularities, LQC has also been used to argue that its quantum geometry effects resolve *all* strong curvature singularities in homogeneous, isotropic situations in which matter is a perfect fluid with an equation of state of the standard type, $p = p(\rho)$ [20]. (For recent reviews, see, e.g., [21,22].) Finally, recent investigations [23,24] of Gowdy models, which have an infinite number of degrees of freedom, also indicate that the big bang is replaced by a quantum bounce.

Detailed and viable quantum theories were constructed in the homogeneous, isotropic case using the so-called ''$\bar{\mu}$'' scheme. A key open question has been whether or not the qualitative features of their Planck scale physics will persist in more realistic situations in which these strong symmetry assumptions do not hold exactly. A first step in this direction is to retain homogeneity and extend the ''improved dynamics'' of [10] to anisotropic situations. In the isotropic case, there is only one nontrivial curvature invariant, the (space-time) scalar curvature (or, equivalently, matter density). In anisotropic situations Weyl curvature is nonzero and it too diverges at the big bang. Therefore, now one can enter the Planck regime in several inequivalent ways which suggests that the Planck scale physics would now be much richer.

In this paper we will continue the LQC explorations of this issue by analyzing in detail the simplest of anisotropic models, the Bianchi type I cosmologies. (Previous work on this model is discussed below.) As in the isotropic case we will use a massless scalar field as the matter source, and it

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will continue to provide the "relational" or "internal" time a la Leibniz with respect to which other physical quantities of interest—e.g., curvatures, shears, expansion, and matter density—"evolve." Again, as in the isotropic case, the framework can be further extended to accommodate additional matter fields in a rather straightforward fashion.

Although the Bianchi I models are the simplest among anisotropic cosmologies, results obtained in the context of the Belinskii, Khalatnikov, Lifshitz (BKL) conjecture [25,26] suggest that they are perhaps the most interesting ones for the issue of singularity resolution. The BKL conjecture states that, as one approaches spacelike singularities in general relativity, terms with time derivatives would dominate over those with spatial derivatives, implying that the asymptotic dynamics would be well described by an ordinary differential equation. By now considerable evidence has accumulated in favor of this conjecture [27–31]. For the case when the matter source is a massless scalar field in full general relativity without any symmetry assumption, these results suggest that, as the system enters the Planck regime, dynamics along any fixed spatial point would be well described by a Bianchi I metric. Therefore understanding the fate of Bianchi I models in LQC could provide substantial intuition for what happens to generic spacelike singularities in LQG [32,33].

Indeed, in cosmological contexts where one has approximate homogeneity, a natural strategy in full LQG is to divide the spatial 3-manifold into small, elementary cells and assume that there is homogeneity in each cell, with fields changing slowly as one moves from one cell to the next. (For an exploration along these lines in the older "μ_o scheme," see [34].) Now, if one were to assume that geometry in each elementary cell is also isotropic, then the Weyl tensor in each cell—and therefore everywhere—would be forced to be zero. A natural strategy to accommodate realistic, nonvanishing Weyl curvature would be to use Bianchi I geometry in each cell and let the parameters characterizing the Bianchi I solution vary slowly from one cell to another. In this manner, LQC of the Bianchi I model can pave way to the analysis of the fate of generic spacelike singularities of general relativity in full LQG.

Because of these potential applications, Bianchi I models have already drawn considerable attention in LQC (see in particular [35–40]). During these investigations, groundwork was laid down which we will use extensively. However, in the spatially noncompact context (i.e., when the spatial topology is $\mathbb{R}^3$ rather than $\mathbb{T}^3$), the construction of the quantum Hamiltonian constraint turned out to be problematic. The Hamiltonian constraint used in the early work has the same difficulties as those encountered in the μ_o scheme in the isotropic case (see, e.g., [12], or Appendix B of [21]). More recent papers have tried to overcome these limitations by mimicking the $\bar{\mu}$ scheme used successfully in the isotropic case. However, to make concrete progress, at a key point in the analysis a simplifying assumption was made without a systematic justification.[1] Unfortunately, it leads to quantum dynamics which depends, even to leading order, on the choice of an auxiliary structure (i.e., the fiducial cell) used in the construction of the Hamiltonian framework [40]. This is a major conceptual drawback. Also, the final results inherit certain features that are not physically viable (e.g., the dependence of the quantum bounce on "directional densities" in [36,37]). We will provide a systematic treatment of quantum dynamics that is free from these drawbacks.

To achieve this goal one has to overcome rather nontrivial obstacles which had stalled progress for the past two years. This requires significant new input. The first is conceptual: we will sharpen the correspondence between LQG and LQC that underlies the definition of the curvature operator $\hat{F}^i_{ab}$ in terms of holonomies. The holonomies we are led to use in this construction will have a nontrivial dependence on triads, stemming from the choice of loops on which they are evaluated. As a result, at first it seems very difficult to define the action of the resulting quantum holonomy operators. Indeed this was the primary technical obstacle that forced earlier investigations to take certain short cuts—the assumption mentioned above—while defining $\hat{F}^i_{ab}$ (see footnote 1). The second new input is the definition of these holonomy operators without having to take a recourse to such short cuts. But then the resulting Hamiltonian constraint appears unwieldy at first. The third major input is a rearrangement of configuration variables that makes the constraint tractable both analytically, as in this paper, and for the numerical work in progress [41].

Finally, we will find that the resulting Hamiltonian constraint has a striking feature which could provide a powerful new tool in relating the quantum dynamics of more complicated models to that of simpler models. It turns out that, in LQC, there is a well-defined projection from the Bianchi I physical states to the Friedmann physical states which maps the Bianchi I quantum dynamics *exactly* to the isotropic quantum dynamics. Previous investigations of the relation between quantum dynamics of a more complicated model to that of a simpler model generally began with an embedding of the Hilbert space $\mathcal{H}_{\mathrm{Res}}$ of the more restricted model in the Hilbert space $\mathcal{H}_{\mathrm{Gen}}$ of the more general model (see, e.g., [42,43]). In generic situations, the image of $\mathcal{H}_{\mathrm{Res}}$ under this embedding was not left invariant by the more general dynamics on $\mathcal{H}_{\mathrm{Gen}}$. This led to a concern that the physics resulting from first re-

[1]In the isotropic case, improved dynamics [10] required that $\bar{\mu}$ be proportional to $1/\sqrt{|p|}$. In the anisotropic case, one has three p_i and quantum dynamics requires the introduction of three $\bar{\mu}_i$. In the Bianchi I case now under consideration, it was simply assumed [36,37,40] that $\bar{\mu}_i$ be proportional to $1/\sqrt{|p_i|}$. We will see in Sec. III B that a more systematic procedure leads to the conclusion that the correct generalization of the isotropic result is more subtle. For example, $\bar{\mu}_1$ is proportional to $\sqrt{|p_1|/|p_2 p_3|}$.

ducing and then quantizing may be completely different from that obtained by quantizing the larger system and regarding the smaller system as its subsystem. The new idea of projecting from $\mathcal{H}_{\rm Gen}$ to $\mathcal{H}_{\rm Res}$ corresponds to ''integrating out the degrees of freedom that are inaccessible to the restricted model'' while the embedding $\mathcal{H}_{\rm Res}$ in to $\mathcal{H}_{\rm Gen}$ corresponds to ''freezing by hand'' these extra degrees of freedom. Classically, both are equally good procedures and in fact the embedding is generally easier to construct. However, in quantum mechanics it is more appropriate to integrate out the extra degrees of freedom. In the present case, one integrates out anisotropies to go from the LQC of the Bianchi I models to that of the Friedmann model. This idea was already proposed and used in [44] in a perturbative treatment of anisotropies in the locally rotationally symmetric, diagonal, Bianchi I model. We extend that work in that we consider the full quantum dynamics of the diagonal Bianchi I model without additional symmetries and, furthermore, use the analog of the $\bar{\mu}$ scheme in which the quantum constraint is considerably more involved than in the μ_o-type scheme used in [44]. The fact that the LQC dynamics of the Friedmann model is recovered exactly provides some concrete support for the hope that LQC may capture the essential features of full LQG, as far as the quantum dynamics of the homogeneous, isotropic degree of freedom is concerned.

The material is organized as follows. We begin in Sec. II with an outline of the classical dynamics of Bianchi type I models. This overview will not be comprehensive as our goal is only to set the stage for the quantum theory which is developed in Sec. III. In Sec. IV we discuss three key properties of quantum dynamics: the projection map mentioned above, agreement of the LQC dynamics with that of the Wheeler-DeWitt (WDW) theory away from the Planck regime, and effective equations. (The isotropic analogs of these equations approximate the full LQC dynamics of Friedmann models extremely well.) In Sec. IV we summarize the main results and discuss some of their ramifications. The Appendix discusses parity-type discrete symmetries which play an important role in the analysis of quantum dynamics.

II. HAMILTONIAN FRAMEWORK

In this section we will summarize those aspects of the classical theory that will be needed for quantization. For a more complete description of the classical dynamics see, e.g., [35–37,45].

Our space-time manifold M will be topologically $\mathbb{R}^4$. As is standard in the literature on Bianchi models, we will restrict ourselves to *diagonal* Bianchi I metrics. Then one can fix Cartesian coordinates τ, x_i on M and express the space-time metric as

$$ds^2 = -N^2 d\tau^2 + a_1^2 dx_1^2 + a_2^2 dx_2^2 + a_3^2 dx_3^2, \qquad (2.1)$$

where N is the lapse and a_i are the directional scale factors. Thus, the dynamical degrees of freedom are encoded in three functions $a_i(\tau)$ of time. Bianchi I symmetries permit us to rescale the three spatial coordinates x_i by independent constants. Under $x_i \to \alpha_i x_i$, the directional scale factors transform as[2] $a_i \to \alpha_i^{-1} a_i$. Thus, the numerical value of a directional scale factor, say a_1, is not an observable; only ratios such as $a_1(\tau)/a_1(\tau')$ are. The matter source will be a massless scalar field which will serve as the relational or internal time. Therefore, it is convenient to work with a harmonic time function, i.e., to ask that τ satisfy $\Box\tau = 0$. From now on we will work with this choice.

Since the spatial manifold is noncompact and all fields are spatially homogeneous, to construct a Lagrangian or a Hamiltonian framework one has to introduce an elementary cell $\mathcal{V}$ and restrict all integrations to it [7]. We will choose $\mathcal{V}$ so that its edges lie along the fixed coordinate axis x_i. As in the isotropic case, it is also convenient to fix a fiducial flat metric ${}^o q_{ab}$ with line element

$$ds_o^2 = dx_1^2 + dx_2^2 + dx_3^2. \qquad (2.2)$$

We will denote by ${}^o q$ the determinant of this metric, by L_i the lengths of the three edges of $\mathcal{V}$ as measured by ${}^o q_{ab}$, and by $V_o = L_1 L_2 L_3$ the volume of the elementary cell $\mathcal{V}$ also measured using ${}^o q_{ab}$. Finally, we introduce fiducial cotriads ${}^o\omega_a^i = D_a x^i$ and the triads ${}^o e_i^a$ dual to them. Clearly they are adapted to the edges of $\mathcal{V}$ and are compatible with ${}^o q_{ab}$ (i.e., satisfy ${}^o q_{ab} = {}^o\omega_a^i {}^o\omega_b^j \delta_{ij}$). As noted above, Bianchi I symmetries allow each of the three coordinates to be rescaled by an independent constant α_i. Under these rescalings, $x_i \to x_i' = \alpha_i x_i$, cotriads transform as ${}^o\omega_a'^i = \alpha_i {}^o\omega_a^i$, and triads ${}^o e_i^a$ are rescaled by inverse powers of α_i. The fiducial metric is transformed to ${}^o q'_{ab}$ defined by $ds_o'^2 := \alpha_1^2 dx_1^2 + \alpha_2^2 dx_2^2 + \alpha_3^2 dx_3^2$. We must ensure that our physical results do not change under these rescalings. Finally, the physical cotriads are given by $\omega_a^i = a^{io}\omega_a^i$ and the physical 3-metric q_{ab} is given by $q_{ab} = \omega_a^i \omega_b^j \delta_{ij}$.

With these fiducial structures at hand, we can now introduce the phase space. Recall first that in LQG the canonical pair consists of an SU(2) connection A_a^i and a triad E_i^a of density weight one. Using the Bianchi I symmetry, from each gauge equivalence class of these pairs we can select one and only one, given by

$$A_a^i =: c^i (L^i)^{-1} {}^o\omega_a^i, \quad \text{and}$$
$$E_i^a \equiv \sqrt{q} e_i^a =: p_i L_i V_o^{-1} \sqrt{{}^o q}\, {}^o e_i^a, \qquad (2.3)$$

where c_i, p_i are constants and $q = (p_1 p_2 p_3) {}^o q V_o^{-1}$ is the determinant of the physical spatial metric q_{ab}. Thus the connections A_a^i are now labeled by three parameters c^i and

[2]Here and in what follows there is no summation over repeated indices if they are all contravariant or all covariant. On the other hand, a covariant index which is contracted with a contravariant one is summed over 1, 2, 3.

the triads E^a_i by three parameters p_i. If p_i are positive, the physical triad e^a_i and the fiducial triad ${}^o e^a_i$ have the same orientation. A change in sign of, say, p_1 corresponds to a change in the orientation of the physical triad brought about by the flip $e^a_1 \to -e^a_1$. These flips are gauge transformations because they do not change the physical metric q_{ab}. The momenta p_i are directly related to the directional scale factors:

$$p_1 = \mathrm{sgn}(a_1)|a_2 a_3| L_2 L_3, \qquad p_2 = \mathrm{sgn}(a_2)|a_1 a_3| L_1 L_3, \qquad p_3 = \mathrm{sgn}(a_3)|a_1 a_2| L_1 L_2, \tag{2.4}$$

where we take the directional scale factor a_i to be positive if the triad vector e^a_i is parallel to ${}^o e^a_i$ and negative if it is antiparallel. As we will see below, in any solution to the field equations, the connection components c_i are directly related to the time derivatives of a_i.

The factors of L_i in (2.3) ensure that this parametrization is unchanged if the fiducial cotriad, triad, and metric are rescaled via $x_i \to \alpha_i x_i$. However, the parametrization does depend on the choice of the cell $\mathcal{V}$. Thus the situation is the same as in the isotropic case [7]. (The physical fields A^i_a and E^a_i are of course insensitive to changes in the fiducial metric *or* the cell.) To evaluate the symplectic structure of the symmetry reduced theory, as in the isotropic case [7], we begin with the expression of the symplectic structure in the full theory and simply restrict the integration to the cell $\mathcal{V}$. The resulting (nonvanishing) Poisson brackets are given by

$$\{c^i, p_j\} = 8\pi G\gamma \delta^i_j. \tag{2.5}$$

To summarize, the phase space in the Bianchi I model is six dimensional, coordinatized by pairs c^i, p_i, subject to the Poisson bracket relations (2.5). This description is tied to the choice of the fiducial cell $\mathcal{V}$ but is insensitive to the choice of fiducial triads, cotriads, and metrics.

Next, let us consider constraints. The full theory has a set of three constraints: the Gauss, the diffeomorphism, and the Hamiltonian constraints. It is straightforward to check that, because we have restricted ourselves to diagonal metrics and fixed the internal gauge, the Gauss and the diffeomorphism constraints are identically satisfied. We are thus left with just the Hamiltonian constraint. Its expression is obtained by restricting the integration in the full theory to the fiducial cell $\mathcal{V}$:

$$\mathcal{C}_H = \mathcal{C}_{\mathrm{grav}} + \mathcal{C}_{\mathrm{matt}} = \int_{\mathcal{V}} N(\mathcal{H}_{\mathrm{grav}} + \mathcal{H}_{\mathrm{matt}}) d^3x, \tag{2.6}$$

where N is the lapse function and the gravitational and the matter parts of the constraint densities are given by

$$\mathcal{H}_{\mathrm{grav}} = \frac{E^a_i E^b_j}{16\pi G\sqrt{|q|}} (\epsilon^{ij}{}_k F_{ab}{}^k - 2(1+\gamma^2) K^i_{[a} K^j_{b]}) \quad \text{and} \quad \mathcal{H}_{\mathrm{matt}} = \sqrt{q}\rho_{\mathrm{matt}}. \tag{2.7}$$

Here γ is the Barbero-Immirzi parameter, and $F_{ab}{}^k$ is the curvature of the connection A^i_a, given by

$$F_{ab}{}^k = 2\partial_{[a} A_{b]}{}^k + \epsilon_{ij}{}^k A^i_a A^j_b, \tag{2.8}$$

K^i_a is related to the extrinsic curvature K_{ab} via $K^i_a = K_{ab} e^{bi}$, and ρ_{matt} is the energy density of the matter fields. In general, A^i_a is related to K^i_a and the spin connection Γ^i_a defined by the triad e^a_i via $A^i_a = \Gamma^i_a + \gamma K^i_a$. However, because Bianchi I models are spatially flat, $\Gamma^i_a = 0$ in the gauge chosen in (2.3), whence $A^i_a = \gamma K^i_a$. This property and the fact that spatial derivatives of K^i_a vanish by the Bianchi I symmetry leads us to the relation

$$2K^i_{[a} K^j_{b]} = \gamma^{-2} \epsilon^{ij}{}_k F_{ab}{}^k. \tag{2.9}$$

Therefore, the gravitational part of the Hamiltonian constraint can be simplified:

$$\begin{aligned} \mathcal{H}_{\mathrm{grav}} &= -\frac{E^a_i E^b_j}{16\pi G\gamma^2\sqrt{q}} \epsilon^{ij}{}_k F_{ab}{}^k \\ &= -\frac{\sqrt{{}^o q}}{8\pi G\gamma^2 \sqrt{p_1 p_2 p_3} V_o} \\ &\quad \times (p_1 p_2 c_1 c_2 + p_1 p_3 c_1 c_3 + p_2 p_3 c_2 c_3). \end{aligned} \tag{2.10}$$

Finally, recall that our matter field is a massless scalar field T. The matter energy density of the scalar field T is given by $\rho_{\mathrm{matt}} = p^2_{(T)}/2V^2$, where $V = \sqrt{|p_1 p_2 p_3|}$ is the physical volume of the elementary cell. Our choice of harmonic time τ implies that the lapse function is given by $N = \sqrt{|p_1 p_2 p_3|}$. With these choices the constraint (2.6) simplifies further:

$$\mathcal{C}_H = \int_{\mathcal{V}} \left(-\frac{E^a_i E^b_j V_o}{16\pi G\gamma^2 \sqrt{{}^o q}} \epsilon_{ij}{}^k F^k_{ab} + \frac{\sqrt{{}^o q}}{V_o} \frac{p^2_T}{2} \right) d^3x \tag{2.11}$$

$$= -\frac{1}{8\pi G\gamma^2} (p_1 p_2 c_1 c_2 + p_1 p_3 c_1 c_3 + p_2 p_3 c_2 c_3) + \frac{p^2_T}{2}. \tag{2.12}$$

Physical states of the classical theory lie on the constraint surface $\mathcal{C}_H = 0$. The time evolution of each p_i and c_i is obtained by taking their Poisson bracket with $\mathcal{C}_H$.

$$\frac{dp_1}{d\tau} = \{p_1, \mathcal{C}_H\} = -8\pi G\gamma \frac{\partial \mathcal{C}_H}{\partial c_1} = \frac{p_1}{\gamma}(p_2 c_2 + p_3 c_3); \tag{2.13}$$

$$\frac{dc_1}{d\tau} = \{c_1, \mathcal{C}_H\} = 8\pi G\gamma \frac{\partial \mathcal{C}_H}{\partial p_1} = \frac{-c_1}{\gamma}(p_2 c_2 + p_3 c_3). \tag{2.14}$$

The four other time derivatives can be obtained via permutations. Although the phase space coordinates c^i, p_i themselves depend on the choice of the fiducial cell $\mathcal{V}$, the

dynamical equations for A_a^i and E_i^a—and hence also for the physical metric q_{ab} and the extrinsic curvature K_{ab}—that follow from (2.13) and (2.14) are independent of this choice.

Combining Eqs. (2.4), (2.13), and (2.14), one finds

$$c_i = \gamma L_i V_o^{-1} (a_1 a_2 a_3)^{-1} \frac{da_i}{d\tau}. \tag{2.15}$$

It is instructive to relate the c_i to the directional Hubble parameters $H_i = d\ln a_i/dt$ where t is the proper time, corresponding to the lapse function $N_{(t)} = 1$. Since t is related to the harmonic time τ via $Nd\tau = N_{(t)}dt$

$$\frac{d}{dt} = \frac{1}{\sqrt{|p_1 p_2 p_3|}} \frac{d}{d\tau}. \tag{2.16}$$

Therefore, we have

$$c_i = \gamma L_i \frac{da_i}{dt} = \gamma L_i a_i H_i, \tag{2.17}$$

where $L_i a_i$ is the length of the ith edge of $\mathcal{V}$ as measured by the physical metric q_{ab}.

Next, it is convenient to introduce a mean scale factor $a := (a_1 a_2 a_3)^{1/3}$ which encodes the physical volume element but ignores anisotropies. Then, the mean Hubble parameter is given by

$$H := \frac{d\ln a}{dt} = \frac{1}{3}(H_1 + H_2 + H_3),$$
$$\text{where as before } H_i := \frac{d\ln a_i}{dt}. \tag{2.18}$$

Squaring Eq. (2.18) and using the implication

$$H_1 H_2 + H_2 H_3 + H_3 H_1 = 8\pi G \rho_{\text{matt}} \tag{2.19}$$

of the Hamiltonian constraint, we obtain the generalized Friedmann equation for Bianchi I space-times,

$$H^2 = \frac{8\pi G}{3}\rho_{\text{matt}} + \frac{\Sigma^2}{a^6}, \tag{2.20}$$

where

$$\Sigma^2 = \frac{a^6}{18}[(H_1 - H_2)^2 + (H_2 - H_3)^2 + (H_3 - H_1)^2] \tag{2.21}$$

is the shear term. The right-hand side of (2.20) brings out the fact that the anisotropic shears $(H_i - H_j)$ contribute to the energy density; they quantify the energy density in the gravitational waves. Using the fact that our matter field has zero anisotropic stress one can show that Σ^2 is a constant of the motion [37]. If the space-time itself is isotropic, then $\Sigma^2 = 0$ and Eq. (2.20) reduces to the usual Friedmann equation for the standard isotropic cosmology. These considerations will be useful in interpreting quantum dynamics and exploring the relation between the Bianchi I and Friedmann quantum Hamiltonian constraints.

Next, let us consider the scalar field T. Because there is no potential for it, its canonically conjugate momentum $p_{(T)}$ is a constant of motion (which, for definiteness, will be assumed to be positive). Therefore, in any solution to the field equations T grows linearly in the harmonic time τ. Thus, although T does not have the physical dimensions of time, it is a good evolution parameter in the classical theory. The form of the quantum Hamiltonian constraint is such that T will also serve as a viable internal time parameter in the quantum theory.

We will conclude with a discussion of discrete "reflection symmetries" that will play an important role in the quantum theory. (For further details see the Appendix.) In the isotropic case, there is a single reflection symmetry, $\Pi(p) = -p$, which physically corresponds to the orientation reversal $e_i^a \to -e_i^a$ of triads. These are large gauge transformations, under which the metric q_{ab} remains unchanged. The Hamiltonian constraint is invariant under this reflection whence one can, if one so wishes, restrict one's attention just to the sector $p \geq 0$ of the phase space. In the Bianchi I case, we have three reflections Π_i, each corresponding to the flip of one of the triad vectors, leaving the other two untouched [e.g., $\Pi_1(p_1, p_2, p_3) = (-p_1, p_2, p_3)$]. As shown in [46], the Hamiltonian flow is left invariant under the action of each Π_i. Therefore, it suffices to restrict one's attention to the positive octant in which all three p_i are non-negative: dynamics in any of the other seven octants can be easily recovered from that in the positive octant by the action of the discrete symmetries Π_i.

Remark.—In the LQC literature on Bianchi I models, a physical distinction has occasionally been made between the fiducial cells $\mathcal{V}$ which are "cubical" with respect to the fiducial metric ${}^o q_{ab}$ and those that are "rectangular." (In the former case all L_i are equal.) However, given *any* cell $\mathcal{V}$ one can always find a flat metric in our collection (2.1) with respect to which that $\mathcal{V}$ is cubical. Using it as ${}^o q_{ab}$ one would be led to call it cubical. Therefore the distinction is unphysical and the hope that the restriction to cubical cells may resolve some of the physical problems faced in [36,37] was misplaced.

III. QUANTUM THEORY

This section is divided into four parts. In the first, we briefly recall quantum kinematics, emphasizing issues that have not been discussed in the literature. In the second, we spell out a simple but well-motivated correspondence between the LQG and LQC quantum states that plays an important role in the definition of the curvature operator $\hat{F}_{ab}{}^k$ in terms of holonomies. However, the paths along which holonomies are evaluated depend in a rather complicated way on the triad (or momentum) operators, whence at first it seems very difficult to define these holonomy operators. In the third section we show that geometric considerations provide a natural avenue to over-

come these apparent obstacles. The resulting Hamiltonian constraint is, however, rather unwieldy to work with. In the last section we make a convenient redefinition of configuration variables to simplify its action. The simplification, in turn, will provide the precise sense in which the singularity is resolved in the quantum theory.

A. LQC kinematics

We will summarize quantum kinematics only briefly; for details, see, e.g., [36,37]. Let us begin by specifying the elementary functions on the classical phase space which are to have unambiguous analogs in the quantum theory. In LQC this choice is directly motivated by the structure of full LQG [1–3]. As one might expect from the isotropic case [7,9], the elementary variables are the three momenta p_i and holonomies $h_i^{(\ell)}$ along edges parallel to the three axis x_i, where ℓL_i is the length of the edge with respect to the fiducial metric ${}^o q_{ab}$.[3] These functions are (over)complete in the sense that they suffice to separate points of the phase space. Taking the x_1 axis for concreteness, the holonomy $h_1^{(\ell)}$ has the form

$$h_1^{(\ell)}(c_1, c_2, c_3) = \cos\frac{c_1\ell}{2}\mathbb{I} + 2\sin\frac{c_1\ell}{2}\tau_1 \tag{3.1}$$

where $\mathbb{I}$ is the unit 2×2 matrix and τ_i constitute a basis of the Lie algebra of SU(2), satisfying $\tau^i\tau^j = \frac{1}{2}\epsilon^{ij}{}_k\tau^k - \frac{1}{4}\delta^{ij}\mathbb{I}$. Thus, the holonomies are completely determined by almost periodic functions $\exp(i\ell c_j)$ of the connection; they are called "almost" periodic because ℓ is any real number rather than an integer. In quantum theory, then, elementary operators $\hat{h}_i^{(\ell)}$ and $\hat{p}_i$ are well defined and our task is to express other operators of physical interest in terms of these elementary ones.

Recall that in the isotropic case it is simplest to specify the gravitational sector of the kinematic Hilbert space in the triad of p representation: it consists of wave functions $\Psi(p)$ which are symmetric under $p \to -p$ and have a finite norm: $\|\Psi\|^2 = \sum_p |\Psi(p)|^2 < \infty$. In the Bianchi I case it is again simplest to describe $\mathcal{H}_{\rm kin}^{\rm grav}$ in the momentum representation. Consider first a *countable* linear combination,

$$|\Psi\rangle = \sum_{p_1,p_2,p_3} \Psi(p_1, p_2, p_3)|p_1, p_2, p_3\rangle \quad \text{with}$$
$$\sum_{p_1,p_2,p_3} |\Psi(p_1, p_2, p_3)|^2 < \infty, \tag{3.2}$$

of orthonormal basis states $|p_1, p_2, p_3\rangle$, where

$$\langle p_1, p_2, p_3|p_1', p_2', p_3'\rangle = \delta_{p_1p_1'}\delta_{p_2p_2'}\delta_{p_3p_3'}. \tag{3.3}$$

Next, recall that on the classical phase space the three reflections Π_i represent large gauge transformations under which physics does not change. They have a natural induced action $\hat{\Pi}_i$ on the space of wave functions $\Psi(p_1, p_2, p_3)$. [Thus, for example, $\hat{\Pi}_1\Psi(p_1, p_2, p_3) = \Psi(-p_1, p_2, p_3)$.] Physical observables commute with $\hat{\Pi}_i$. Therefore, as in gauge theories, each eigenspace of $\hat{\Pi}_i$ provides a physical sector of the theory. Since $\hat{\Pi}_i^2 = \mathbb{I}$, eigenvalues of $\hat{\Pi}_i$ are ± 1. For definiteness, as in the isotropic case, we will assume that the wave functions $\Psi(p_1, p_2, p_3)$ are symmetric under $\hat{\Pi}_i$. Thus, the gravitational part $\mathcal{H}_{\rm kin}^{\rm grav}$ of the kinematical Hilbert space is spanned by wave functions $\Psi(p_1, p_2, p_3)$ satisfying

$$\Psi(p_1, p_2, p_3) = \Psi(|p_1|, |p_2|, |p_3|) \tag{3.4}$$

which have finite norm (3.2).

The basis states $|p_1, p_2, p_3\rangle$ are eigenstates of quantum geometry: In the state $|p_1, p_2, p_3\rangle$ the face S_i of the fiducial cell $\mathcal{V}$ orthogonal to the axis x_i has area $|p_i|$. Note that although $p_i \in \mathbb{R}$, the orthonormality holds via Kronecker deltas rather than the usual Dirac distributions; this is why the LQC quantum kinematics is inequivalent to that of the Schrödinger theory used in Wheeler-DeWitt cosmology. Finally the action of the elementary operators is given by

$$\hat{p}_1|p_1, p_2, p_3\rangle = p_1|p_1, p_2, p_3\rangle \quad \text{and}$$
$$\widehat{\exp i\ell c_1}|p_1, p_2, p_3\rangle = |p_1 - 8\pi\gamma G\hbar\ell, p_2, p_3\rangle \tag{3.5}$$

and similarly for $\hat{p}_2$, $\widehat{\exp i\ell c_2}$, $\hat{p}_3$, and $\widehat{\exp i\ell c_3}$.

The full kinematical Hilbert space $\mathcal{H}_{\rm kin}$ will be the tensor product, $\mathcal{H}_{\rm kin} = \mathcal{H}_{\rm kin}^{\rm grav} \otimes \mathcal{H}_{\rm kin}^{\rm matt}$ where, as in the isotropic case, we will set $\mathcal{H}_{\rm kin}^{\rm matt} = L^2(\mathbb{R}, dT)$ for the Hilbert space of the homogeneous scalar field T. On $\mathcal{H}_{\rm kin}^{\rm matt}$, the operator $\hat{T}$ will act by multiplication and $\hat{p}_{(T)} := -i\hbar d/dT$ will act by differentiation. Note that we can also use a "polymer Hilbert space" for $\mathcal{H}_{\rm kin}^{\rm matt}$ spanned by almost periodic functions of T. The quantum Hamiltonian constraint (3.22) will remain unchanged and our construction of the physical Hilbert space will go through as it is [47].

B. The curvature operator $\hat{F}_{ab}{}^k$

To discuss quantum dynamics, we have to construct the quantum analog of the Hamiltonian constraint. Since there is no operator corresponding to the connection coefficients c_i on $\mathcal{H}_{\rm kin}^{\rm grav}$, we cannot use (2.12) directly. Rather, as in the isotropic case [10], we will return to the expression (2.11) involving curvature $F_{ab}{}^k$. Our task then is to find the operator on $\mathcal{H}_{\rm kin}^{\rm grav}$ corresponding to $F_{ab}{}^k$. As is usual in LQG, the idea is to first express the curvature in terms of our elementary variables—holonomies and triads—and

[3] More precisely, the dimensionless number ℓ is the length of the edge along which the holonomy is evaluated, measured in the units of the length of the edge of $\mathcal{V}$ parallel to it. Since ℓ is a ratio of lengths, its value does not depend on the fiducial or any other metric.

then replace them by their direct quantum analogs. Recall first that, in the classical theory, the a-b component of ${F_{ab}}^k$ can be written in terms of holonomies around a plaquette (i.e., a rectangular closed loop whose edges are parallel to two of the axes x_i):

$$ {F_{ab}}^k = 2 \lim_{Ar_\square \to 0} \mathrm{Tr}\left(\frac{h_{\square_{ij}} - \mathbb{I}}{Ar_\square} \tau^k \right) {}^o\omega_a^i \, {}^o\omega_b^j, \tag{3.6} $$

where $Ar_\square$ is the area of the plaquette $\square$ and the holonomy $h_{\square_{ij}}$ around the plaquette $\square_{ij}$ is given by

$$ h_{\square_{ij}} = h_j^{(\bar{\mu}_j)^{-1}} h_i^{(\bar{\mu}_i)^{-1}} h_j^{(\bar{\mu}_j)} h_i^{(\bar{\mu}_i)}, \tag{3.7} $$

where $\bar{\mu}_j L_j$ is the length of the jth edge of the plaquette, as measured by the fiducial metric ${}^oq_{ab}$. (There is no summation over i, j.) Because the $Ar_\square$ is shrunk to zero, the limit is not sensitive to the precise choice of the closed plaquette $\square$. Now, in LQG the connection operator does not exist, whence if we regard the right side of (3.6) as an operator, the limit fails to converge in $\mathcal{H}^{\mathrm{grav}}_{\mathrm{kin}}$. The nonexistence of the connection operator is a direct consequence of the underlying diffeomorphism invariance [48] and is intertwined with the fact that the eigenvalues of geometric operators—such as the area operator $\widehat{Ar}_\square$ associated with the plaquette under consideration—are purely discrete. Therefore, in LQC the viewpoint is that the nonexistence of the limit $Ar_\square \to 0$ in quantum theory is not accidental: quantum geometry is simply telling us that we should shrink the plaquette not till the area it encloses goes to zero, but rather only to the minimum nonzero eigenvalue $\Delta \ell_{\mathrm{Pl}}^2$ of the area operator (where Δ is a dimensionless number). The resulting quantum operator ${\hat{F}_{ab}}^k$ then inherits Planck scale nonlocalities.

To implement this strategy in full LQG one must resolve a difficult issue. If the plaquette is to be shrunk only to a finite size, the operator on the right side of (3.6) would depend on what that limiting plaquette is. So, which of the many plaquettes enclosing an area $\Delta \ell_{\mathrm{Pl}}^2$ should one use? Without a well-controlled gauge fixing procedure, it would be very difficult to single out such plaquettes, one for each 2-dimensional plane in the tangent space at each spatial point. However, in the diagonal Bianchi I case now under consideration, a natural gauge fixing is available and indeed we have already carried it out. Thus, in the i-j plane, it is natural to choose a plaquette $\square_{ij}$ so that its edges are parallel to the x_i-x_j axis. Furthermore, the underlying homogeneity implies that it suffices to introduce the three plaquettes at any one point in our spatial 3-manifold.

These considerations severely limit the choice of plaquettes $\square_{ij}$ but they do not determine the lengths of the two edges in each of these plaquettes. To completely determine the plaquettes, as in the isotropic case, we will use a simple but well-motivated correspondence between kinematic states in LQG and those in LQC. However, because of anisotropies, new complications arise which require that the correspondence be made much more precise. Fix a state $|p_1, p_2, p_3\rangle$ in $\mathcal{H}^{\mathrm{grav}}_{\mathrm{kin}}$ of LQC. In this state, the three faces of the fiducial cell $\mathcal{V}$ orthogonal to the x_i axis have areas $|p_i|$ in the LQC *quantum* geometry. This is the complete physical information in the ket $|p_1, p_2, p_3\rangle$. How would this quantum geometry be represented in full LQG? First, the macroscopic geometry must be spatially homogeneous and we have singled out three axes with respect to which our metrics are diagonal. Therefore, semiheuristic considerations suggest that the corresponding LQG quantum geometry state should be represented by a spin network consisting of edges parallel to the three axes [see Fig. 1(a)]. Microscopically this state is not exactly homogeneous. But the *coarse grained* geometry should be homogeneous. To achieve the best possible coarse grained homogeneity, the edges should be packed as tightly as is possible in the desired quantum geometry. That is, each edge should carry the smallest nonzero label possible, namely, $j = 1/2$.

For definiteness, let us consider the 1-2 face S_{12} of the fiducial cell $\mathcal{V}$ which is orthogonal to the x_3 axis [see Fig. 1(b)]. Quantum geometry of LQG tells us that at each intersection of any one of its edges with S_{12}, the spin network contributes a quantum of area $\Delta \ell_{\mathrm{Pl}}^2$ on this surface, where $\Delta = 4\pi\gamma\sqrt{3}$ [49]. For this LQG state to reproduce the LQC state $|p_1, p_2, p_3\rangle$ under consideration, S_{12} must be pierced by N_3 edges of the LQG spin network, where N_3 is given by

$$ N_3 \Delta \ell_{\mathrm{Pl}}^2 = |p_3|. $$

Thus, we can divide S_{12} into N_3 identical rectangles each of which is pierced by exactly one edge of the LQG state, as in Fig. 1(b). Any one of these elementary rectangles encloses an area $\Delta \ell_{\mathrm{Pl}}^2$ and provides us the required plaquette $\square_{12}$. Let the dimensionless lengths of the edges of these plaquettes be $\bar{\mu}_1$ and $\bar{\mu}_2$. Then their lengths with respect to the fiducial metric ${}^oq_{ab}$ are $\bar{\mu}_1 L_1$ and $\bar{\mu}_2 L_2$.

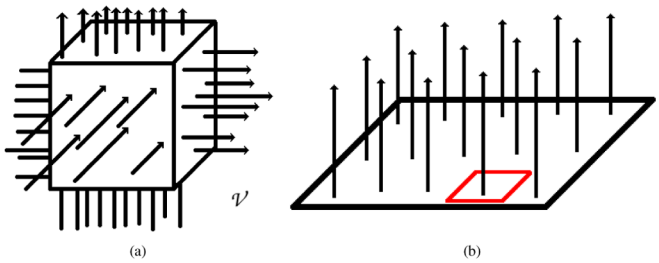

FIG. 1 (color online). Depiction of the LQG quantum geometry state corresponding to the LQC state $|p_1, p_2, p_3\rangle$. The LQG spin network has edges parallel to the three axes selected by the diagonal Bianchi I symmetries, each carrying a spin label $j = 1/2$. (a) Edges of the spin network traversing through the fiducial cell $\mathcal{V}$. (b) Edges of the spin network traversing the 1-2 face of $\mathcal{V}$ and an elementary plaquette associated with a single flux line. This plaquette encloses the smallest quantum, $\Delta \ell_{\mathrm{Pl}}^2$, of area. The curvature operator ${\hat{F}_{12}}^k$ is defined by the holonomy around such a plaquette.

Since the area of S_{12} with respect to ${}^o q_{ab}$ is $L_1 L_2$, we have

$$N_3 \bar{\mu}_1 L_1 \bar{\mu}_2 L_2 = L_1 L_2.$$

Equating the expressions of N_3 from the last two equations, we obtain

$$\bar{\mu}_1 \bar{\mu}_2 = \frac{\Delta \ell_{\rm Pl}^2}{|p_3|}. \tag{3.8}$$

This relation by itself does not fix $\bar{\mu}_1$ and $\bar{\mu}_2$. However, repeating this procedure for the 2-3 face and the 3-1 face, we obtain, in addition, two cyclic permutations of this last equation and the three simultaneous equations do suffice to determine $\bar{\mu}_i$:

$$\bar{\mu}_1 = \sqrt{\frac{|p_1|\Delta \ell_{\rm Pl}^2}{|p_2 p_3|}}, \qquad \bar{\mu}_2 = \sqrt{\frac{|p_2|\Delta \ell_{\rm Pl}^2}{|p_1 p_3|}}, \qquad \bar{\mu}_3 = \sqrt{\frac{|p_3|\Delta \ell_{\rm Pl}^2}{|p_1 p_2|}}. \tag{3.9}$$

To summarize, by exploiting the Bianchi I symmetries and using a simple but well-motivated correspondence between LQG and LQC states we have determined the required elementary plaquettes enclosing an area $\Delta \ell_{\rm Pl}^2$ on each of the three faces of the cell $\mathcal{V}$. On the face S_{ij}, the plaquette is a rectangle whose sides are parallel to the x_i and x_j axes and whose dimensionless lengths are $\bar{\mu}_i$ and $\bar{\mu}_j$, respectively, given by (3.9). Note that (as in the isotropic case [10]) the $\bar{\mu}_i$ and hence the plaquettes are not fixed once and for all; they depend on the LQC state $|p_1, p_2, p_3\rangle$ of quantum geometry in a specific fashion. The functional form of this dependence is crucial to ensure that the resulting quantum dynamics is free from the difficulties encountered in earlier works.

Components of the curvature operator $\hat{F}_{ab}{}^k$ can now be expressed in terms of holonomies around these plaquettes:

$$\hat{F}_{ab}{}^k = 2 \sum_{i,j} \mathrm{Tr}\left(\frac{h_{\Box_{ij}} - \mathbb{I}}{\bar{\mu}_i \bar{\mu}_j L_i L_j} \tau^k \right) {}^o\omega_a^i \, {}^o\omega_b^j, \tag{3.10}$$

with

$$h_{\Box_{ij}} = h_j^{(\bar{\mu}_j)^{-1}} h_i^{(\bar{\mu}_i)^{-1}} h_j^{(\bar{\mu}_j)} h_i^{(\bar{\mu}_i)}, \tag{3.11}$$

where $\bar{\mu}_j$ are given by (3.9). (There is no summation over i, j.) Using the expression (3.1) of holonomies, it is straightforward to evaluate the right-hand side. One finds

$$\hat{F}_{ab}{}^k = \epsilon_{ij}{}^k \left(\frac{\sin \bar{\mu} c}{\bar{\mu} L} {}^o\omega_a \right)^i \left(\frac{\sin \bar{\mu} c}{\bar{\mu} L} {}^o\omega_b \right)^j, \tag{3.12}$$

where the usual summation convention for repeated covariant and contravariant indices applies and

$$\left(\frac{\sin \bar{\mu} c}{\bar{\mu} L} {}^o\omega_a \right)^i = \frac{\sin \bar{\mu}^i c^i}{\bar{\mu}^i L^i} {}^o\omega_a^i, \tag{3.13}$$

where there is now no sum over i. This is the curvature operator we were seeking.

We will conclude with a discussion of the important features of this procedure and of the resulting quantum dynamics.

(1) In the isotropic case all p_i are equal ($p_i = p$) whence our expressions for $\bar{\mu}_i$ reduce to a single formula, $\bar{\mu} = \sqrt{\Delta \ell_{\rm Pl}^2 / |p|}$. This is precisely the result that was obtained in the improved dynamics scheme for the $k = 0$ isotropic models. Thus, we have obtained a generalization of that result to Bianchi I models.

(2) In both cases, the key observation is that the plaquette should be shrunk till its area with respect to the physical—rather than the fiducial—geometry is $\Delta \ell_{\rm Pl}^2$. However, there are also some differences. First, in the above analysis we set up and used a correspondence between quantum geometries of LQG and LQC in the context of Bianchi I models. In contrast to the previous treatment in the isotropic models [10], we did not have to bring in classical geometry in the intermediate steps. In this sense, even for the isotropic case, the current analysis is an improvement over what is available in the literature.

(3) A second difference between our present analysis and that of [10] is the following. Here, the semi-heuristic representation of LQC states $|p_1, p_2, p_3\rangle$ in terms of spin networks of LQG suggested that we should consider spin networks which pierce the faces of the fiducial cell $\mathcal{V}$ as in Fig. 1(a). (As one would expect, these states are gauge invariant.) The minimum nonzero eigenvalue of the area operator on such states is $\Delta \ell_{\rm Pl}^2$ with $\Delta = 4\sqrt{3}\pi\gamma$. This is *twice* the absolute minimum of nonzero eigenvalue on *all* gauge invariant states. However, that lower value is achieved on spin networks (whose edges are again labeled by $j = 1/2$ but) which do not pierce the surface but rather intersect it from only one side. (In order for the state to be gauge invariant, the edge then has to continue along a direction tangential to the surface. For details, see [49].) Obvious considerations suggest that such states cannot feature in homogeneous models. Since the discussion in the isotropic case invoked a correspondence between LQG and LQC at a rougher level, this point was not noticed and the value of Δ used in [10] was $2\sqrt{3}\pi\gamma$. We emphasize, however, that although the current discussion is more refined, it is not a self-contained derivation. A more complete analysis may well change this numerical factor again.

(4) On the other hand, we believe that the functional dependence of $\bar{\mu}_i$ on p_i is robust: As in the isotropic case this dependence appears to be essential to make quantum dynamics viable. Otherwise quantum dy-

namics can either depend on the choice of the fiducial cell $\mathcal{V}$ even to leading order, or is physically incorrect because it allows quantum effects to dominate in otherwise "tame" situations, or both. The previous detailed, quantum treatments of the Bianchi I model in LQC did not have this functional dependence because they lacked the correspondence between LQG and LQC we used. Rather, they proceeded by analogy. As we noted above, in the isotropic case there is a single $\bar{\mu}$ and a single p and the two are related by $\bar{\mu} = \sqrt{\Delta \ell_{\rm Pl}^2/|p|}$. The most straightforward generalization of this relation to Bianchi I models is $\bar{\mu}_i = \sqrt{\Delta \ell_{\rm Pl}^2/|p_i|}$. This expression was simply postulated and then used to construct quantum dynamics [36,37]. The resulting analysis has provided a number of useful technical insights. However, this quantum dynamics suffers from the problems mentioned above [40]. The possibility that the correct generalization of the isotropic results to Bianchi I models may be given by (3.9) was noted in [38,50] and in Appendix C of [37]. However, for reasons explained in the next section, construction of the quantum Hamiltonian operator based on (3.9) was thought not to be feasible. Therefore, this avenue was used only to gain qualitative insights and was not pursued in the full quantum theory.

C. The quantum Hamiltonian constraint

With the curvature operator $\hat{F}_{ab}{}^{k}$ at hand, it is straightforward to construct the quantum analog of the Hamiltonian constraint (2.6) because the triad operators can be readily constructed from the three $\hat{p}_i$. Ignoring for a moment the factor ordering issues, the gravitational part of this operator is given by

$$\begin{aligned}\hat{\mathcal{C}}_{\rm grav} = &-\frac{1}{8\pi G\gamma^2\Delta\ell_{\rm Pl}^2}[p_1p_2|p_3|\sin\bar{\mu}_1c_1\sin\bar{\mu}_2c_2\\ &+ p_1|p_2|p_3\sin\bar{\mu}_1c_1\sin\bar{\mu}_3c_3\\ &+ |p_1|p_2p_3\sin\bar{\mu}_2c_2\sin\bar{\mu}_3c_3],\end{aligned} \tag{3.14}$$

where for simplicity of notation here and in what follows we have dropped hats on p_i and $\sin\bar{\mu}_ic_i$. To write the action of this operator on $\mathcal{H}_{\rm kin}^{\rm grav}$, it suffices to specify the action of the operators $\exp(i\bar{\mu}_ic_i)$ on the kinematical states $\Psi(p_1, p_2, p_3)$. The expression (3.9) of $\bar{\mu}_i$ and the Poisson brackets (2.5) imply

$$\exp(\pm i\bar{\mu}_1c_1) = \exp\left(\mp 8\pi\gamma\sqrt{\Delta}\ell_{\rm Pl}^3\sqrt{\left|\frac{p_1}{p_2p_3}\right|}\,\frac{d}{dp_1}\right) \tag{3.15}$$

and its cyclic permutations. At first sight this expression seems too complicated to yield a manageable Hamiltonian constraint.

Remark.—In the isotropic case, the corresponding expression is simply

$$\exp(\pm i\bar{\mu}c) = \exp\left(\mp 8\pi\gamma\sqrt{\Delta}\ell_{\rm Pl}^3\sqrt{\left|\frac{1}{p}\right|}\,\frac{d}{dp}\right).$$

Since $\frac{1}{\sqrt{p}}\frac{d}{dp} \sim \frac{d}{dv}$, where $v \sim |p|^{3/2}$ is the physical volume of the fiducial cell $\mathcal{V}$, this operator can be essentially written as $\exp(d/dv)$ and acts just as a displacement operator on functions $\Psi(v)$ of v. In the operator (3.15) by contrast, all three p_i feature in the exponent. This is why its action was deemed unmanageable. As we noted at the end of Sec. III B, progress was made [36,37] by simply postulating an alternative, more manageable expression $\bar{\mu}_i = (\sqrt{\Delta}\ell_{\rm Pl}/\sqrt{|p_i|})$, the obvious analog of $\bar{\mu} = (\sqrt{\Delta}\ell_{\rm Pl})/\sqrt{|p|}$ in the isotropic case [10]. Then each $\exp(\pm i\bar{\mu}_ic_i)$ can be expressed essentially as a displacement operator $\exp(d/dv_i)$ with $v_i \sim |p_i|^{3/2}$ and the procedure used in the isotropic case could be implemented on states $\Psi(v_1, v_2, v_3)$. Bianchi I quantum dynamics then resembled three copies of the isotropic dynamics. However, as noted above this solution is not viable [40].

Our new observation is that the operator (3.15) can in fact be handled in a manageable fashion. Let us first make an algebraic simplification by introducing new dimensionless variables λ_i:

$$\lambda_i = \frac{\mathrm{sgn}(p_i)\sqrt{|p_i|}}{(4\pi|\gamma|\sqrt{\Delta}\ell_{\rm Pl}^3)^{1/3}}, \tag{3.16}$$

[so that $\mathrm{sgn}(\lambda_i) = \mathrm{sgn}(p_i)$]. Then, we can introduce a new orthonormal basis $|\lambda_1, \lambda_2, \lambda_3\rangle$ in $\mathcal{H}_{\rm kin}^{\rm grav}$ by an obvious rescaling. These vectors are again eigenvectors of the operators p_i:

$$p_i|\lambda_1, \lambda_2, \lambda_3\rangle = \mathrm{sgn}(\lambda_i)(4\pi|\gamma|\sqrt{\Delta}\ell_{\rm Pl}^3)^{2/3}\lambda_i^2|\lambda_1, \lambda_2, \lambda_3\rangle. \tag{3.17}$$

We can expand out any ket $|\Psi\rangle$ in $\mathcal{H}_{\rm kin}^{\rm grav}$ as $|\Psi\rangle = \Psi(\lambda_1, \lambda_2, \lambda_3)|\lambda_1, \lambda_2, \lambda_3\rangle$ and reexpress the right side of (3.15) as an operator on wave functions $\Psi(\vec{\lambda})$,

$$\exp(\pm i\bar{\mu}_1c_1) = \exp\left(\frac{\mp\mathrm{sgn}(\lambda_1)}{\lambda_2\lambda_3}\,\frac{d}{d\lambda_1}\right) =: E_1^{\mp}, \tag{3.18}$$

where the notation $E_i^{\pm}$ has been introduced as shorthand. [Here, we have used the property $\gamma = \mathrm{sgn}(p_1p_2p_3)|\gamma|$ of the Barbero-Immirzi parameter from the Appendix.] To obtain the explicit action of $E_i^{\pm}$ on wave functions $\Psi(\vec{\lambda})$ we note that, since the operator is an exponential of a vector field, its action is simply to drag the wave function $\Psi(\vec{\lambda})$ a unit affine parameter along its integral curves. Furthermore, since the vector field $d/d\lambda_1$ is in the λ_1 direction, the coefficient $1/\lambda_2\lambda_3$ is constant along each

of its integral curves. Therefore it is possible to write down the explicit expression of $E_i^{\pm}$:

$$(E_1^{\pm}\Psi)(\lambda_1, \lambda_2, \lambda_3) = \Psi\Big(\lambda_1 \pm \frac{\mathrm{sgn}(\lambda_1)}{\lambda_2\lambda_3}, \lambda_2, \lambda_3\Big). \quad (3.19)$$

The nontriviality of this action lies in the fact that while the wave function is dragged along the λ_1 direction, the affine distance involved in this dragging depends on λ_2, λ_3. This operator is well defined because our states have support only on a countable number of λ_i. In particular, the image $(E_1^{\pm}\Psi)(\vec{\lambda})$ vanishes identically at points $\lambda_2 = 0$ or $\lambda_3 = 0$ because Ψ does not have support at $\lambda_1 = \infty$. Thus the factor $\lambda_2\lambda_3$ appearing in the denominator does not cause difficulties.

We can now write out the gravitational part of the Hamiltonian constraint:

$$\hat{\mathcal{C}}_{\mathrm{grav}} = \hat{\mathcal{C}}^{(1)}_{\mathrm{grav}} + \hat{\mathcal{C}}^{(2)}_{\mathrm{grav}} + \hat{\mathcal{C}}^{(3)}_{\mathrm{grav}}, \quad (3.20)$$

with

$$\begin{aligned}\hat{\mathcal{C}}^{(1)}_{\mathrm{grav}} = &-\pi\hbar\ell_{\mathrm{Pl}}^2\sqrt{|\lambda_1\lambda_2\lambda_3|}[\sin\bar{\mu}_2 c_2\, \mathrm{sgn}\lambda_2|\lambda_1\lambda_2\lambda_3|\mathrm{sgn}\lambda_3 \\ &\times \sin\bar{\mu}_3 c_3 + \sin\bar{\mu}_3 c_3\, \mathrm{sgn}\lambda_3|\lambda_1\lambda_2\lambda_3|\mathrm{sgn}\lambda_2 \\ &\times \sin\bar{\mu}_2 c_2]\sqrt{|\lambda_1\lambda_2\lambda_3|}, \end{aligned} \quad (3.21)$$

where we have used the simplest symmetric factor ordering that reduces to the one used in [11] in the isotropic case. ($\hat{\mathcal{C}}^{(2)}_{\mathrm{grav}}$ and $\hat{\mathcal{C}}^{(3)}_{\mathrm{grav}}$ are given by the obvious cyclic permutations.) In the Appendix, we show that, under the action of reflections $\hat{\Pi}_i$ on $\mathcal{H}^{\mathrm{grav}}_{\mathrm{kin}}$, the operators $\sin\bar{\mu}_i c_i$ have the same transformation properties that c_i have under reflections Π_i in the classical theory. As a consequence, $\hat{\mathcal{C}}_{\mathrm{grav}}$ is also reflection symmetric. Therefore, its action is well defined on $\mathcal{H}^{\mathrm{grav}}_{\mathrm{kin}}$: $\hat{\mathcal{C}}_{\mathrm{grav}}$ is a densely defined, symmetric operator on this Hilbert space. In the isotropic case, its analog has been shown to be essentially self-adjoint [51]. In what follows we will assume that (3.20) is essentially self-adjoint on $\mathcal{H}^{\mathrm{grav}}_{\mathrm{kin}}$ and work with its self-adjoint extension.

Finally, it is straightforward to write down the quantum analog of the full Hamiltonian constraint (2.6):

$$-\hbar^2\partial_T^2\Psi(\vec{\lambda}, T) = \Theta\Psi(\vec{\lambda}, T), \quad (3.22)$$

where $\Theta = -\mathcal{C}_{\mathrm{grav}}$. As in the isotropic case, one can obtain the physical Hilbert space $\mathcal{H}_{\mathrm{phy}}$ by a group averaging procedure and the result is completely analogous. Elements of $\mathcal{H}_{\mathrm{phy}}$ consist of "positive frequency" solutions to (3.22), i.e., solutions to

$$-i\hbar\partial_T\Psi(\vec{\lambda}, T) = \sqrt{|\Theta|}\Psi(\vec{\lambda}, T), \quad (3.23)$$

which are symmetric under the three reflection maps $\hat{\Pi}_i$, i.e., satisfy

$$\Psi(\lambda_1, \lambda_2, \lambda_3, T) = \Psi(|\lambda_1|, |\lambda_2|, |\lambda_3|, T). \quad (3.24)$$

The scalar product is given simply by

$$\begin{aligned}\langle\Psi_1|\Psi_2\rangle &= \langle\Psi_1(\vec{\lambda}, T_o)|\Psi_2(\vec{\lambda}, T_o)\rangle_{\mathrm{kin}} \\ &= \sum_{\lambda_1,\lambda_2,\lambda_3}\bar{\Psi}_1(\vec{\lambda}, T_o)\Psi_2(\vec{\lambda}, T_o), \end{aligned} \quad (3.25)$$

where T_o is any "instant" of internal time T.

Remark.—In the isotropic LQC literature [10,16,17] one began in the classical theory with proper time t (which corresponds to the lapse function $N_{(t)} = 1$) and made a transition to the relational time provided by the scalar field only in the construction of the physical sector of the quantum theory. If we had used that procedure here, the factor ordering of the Hamiltonian constraint would have been slightly different. In this paper, we started out with the lapse $N = |p_1p_2p_3|^{1/2}$ already in the classical theory because the resulting quantum Hamiltonian constraint is simpler. In the isotropic case, for example, this procedure leads to an *analytically soluble* model (the one obtained in [11] by first starting out with $N_{(t)} = 1$, then going to quantum theory, and finally making some well-motivated but simplifying assumptions). It also has some conceptual advantages because it avoids the use of "inverse scale factors" altogether.

D. Simplification of $\hat{\mathcal{C}}_{\mathrm{grav}}$

It is straightforward to expand out the Hamiltonian constraint $\hat{\mathcal{C}}_{\mathrm{grav}}$ using the explicit action of operators $\sin(\bar{\mu}_i c_i)$ given by (3.19) and express it as a linear combination of 24 terms of the type

$$\hat{\mathcal{C}}^{\pm\pm}_{ij} := \sqrt{|v|}E_i^{\pm}\,\mathrm{sgn}(\lambda_i)|v|\mathrm{sgn}(\lambda_j)E_j^{\pm}\sqrt{|v|}, \quad (3.26)$$

(where $i \neq j$ and as before there is no summation over i, j). Unfortunately, the $\mathrm{sgn}(\lambda_i)$ factors in this expression and in the action of $E_i^{\pm}$ make the result quite complicated. More importantly, it is rather difficult to interpret the resulting operator. The expression can be simplified if we introduce the volume of $\mathcal{V}$ as one of the arguments of the wave function. In particular, this would make quantum dynamics easier to compare with that of the Friedmann models. With this motivation, let us further rearrange the configuration variables and set

$$v = 2\lambda_1\lambda_2\lambda_3. \quad (3.27)$$

The factor of 2 in (3.27) ensures that this v reduces to the v used in the isotropic analysis of [10] (if one uses the value of Δ used there). As the notation suggests, v is directly related to the volume of the elementary cell $\mathcal{V}$:

$$\hat{V}\Psi(\lambda_1, \lambda_2, v) = 2\pi|\gamma|\sqrt{\Delta}|v|\ell_{\mathrm{Pl}}^3\Psi(\lambda_1, \lambda_2, v). \quad (3.28)$$

One's first impulse would be to introduce two other variables in a symmetric fashion, e.g., following Misner [52].

Unfortunately, detailed examination shows that they make the constraint (3.20) even less transparent.[4]

Let us simply use λ_1, λ_2, and v as the configuration variables in place of λ_1, λ_2, and λ_3. This change of variables would be nontrivial in the Schrödinger representation but is completely tame here because the norms on $\mathcal{H}^{\rm grav}_{\rm kin}$ are defined using a discrete measure on $\mathbb{R}^3$. As a consequence, the scalar product is again given by the sum in (3.25), the only difference is that λ_3 is now replaced by v. Since the choice $(\lambda_1, \lambda_2, v)$ breaks the permutation symmetry, one might have first thought that it would not be appropriate. Somewhat surprisingly, as we will now show, it suffices to make the structure of the constraint transparent. (Of course, the simplification of the constraint would have persisted if we had chosen to replace either λ_1 or λ_2—rather than λ_3—with v.) Finally, note that the positive octant is now given by $\lambda_1 \geq 0$, $\lambda_2 \geq 0$, and $v \geq 0$.

To obtain the explicit action of the constraint, it is extremely convenient to use the fact that states Ψ in $\mathcal{H}^{\rm grav}_{\rm kin}$ satisfy the symmetry condition (3.24) and that $\hat{\mathcal{C}}_{\rm grav}$ has a well-defined action on this space. Therefore, to specify its action on any given Ψ it suffices to find the restriction of the image $\Phi(\lambda_1, \lambda_2, v) := (\hat{\mathcal{C}}_{\rm grav}\Psi)(\lambda_1, \lambda_2, v)$ to the positive octant. The value of Φ in other octants is determined by its symmetry property. This fact greatly simplifies our task because we can use it to eliminate the $\mathrm{sgn}(\lambda_i)$ factors in various terms which complicate the expression tremendously.

For concreteness let us focus on one term in the constraint operator (which turns out to be the most nontrivial one for our simplification):

$$\begin{aligned}(\hat{\mathcal{C}}^{--}_{21}\Psi)(\lambda_1, \lambda_2, v) &:= (\sqrt{|v|}E^-_2\,\mathrm{sgn}(\lambda_2)|v|\mathrm{sgn}(\lambda_1)E^-_1\sqrt{|v|}\Psi)(\lambda_1, \lambda_2, v)\\ &= \left[\sqrt{|v|}\,\mathrm{sgn}\left(\lambda_2\left(1-\frac{2\,\mathrm{sgn}\lambda_2}{v}\right)\right)|v-2\,\mathrm{sgn}\lambda_2|\mathrm{sgn}(\lambda_1)\sqrt{|v-2\,\mathrm{sgn}\lambda_1-2\,\mathrm{sgn}\lambda_2|}\right]\\ &\quad\times\Psi\left(\frac{v-2\,\mathrm{sgn}\lambda_1-2\,\mathrm{sgn}\lambda_2}{v-2\,\mathrm{sgn}\lambda_2}\lambda_1, \frac{v-2\,\mathrm{sgn}\lambda_2}{v}\lambda_2, v-2\,\mathrm{sgn}\lambda_1-2\mathrm{sgn}\lambda_2\right).\end{aligned} \tag{3.29}$$

If we now restrict the argument of $(\hat{\mathcal{C}}^{--}_{12}\Psi)$ to the positive octant, the expression simplifies:

$$\begin{aligned}(\hat{\mathcal{C}}^{--}_{21}\Psi)|_{+\rm octant} &= [\sqrt{v}(v-2)\sqrt{|v-4|}]\\ &\quad\times\Psi\left(\frac{v-4}{v-2}\lambda_1, \frac{v-2}{v}\lambda_2, v-4\right).\end{aligned} \tag{3.30}$$

Now the action of this operator is more transparent: the wave function is multiplied by functions *only* of volume and, in the argument of the wave function, volume simply shifts by -4 and λ_1, λ_2 are rescaled by multiplicative factors which also depend *only* on the volume. Since the full constraint is a linear combination of terms of this form, its action is also driven primarily by volume. As we will see, this key property makes the constraint manageable and greatly simplifies the task of analyzing the relation between the LQC quantum dynamics of Bianchi I and Friedmann models. From now on, unless otherwise stated, we will restrict the argument of the images $(\hat{\mathcal{C}}^{\pm}_{ij}\Psi)$ to lie in the positive octant; its value in other octants is given simply by $(\hat{\mathcal{C}}^{\pm\pm}_{ij}\Psi)(\lambda_1, \lambda_2, v) = (\hat{\mathcal{C}}^{\pm\pm}_{ij}\Psi)(|\lambda_1|, |\lambda_2|, |v|)$.

The form (3.30) of the action of operators $\hat{\mathcal{C}}^{\pm\pm}_{ij}$ enables us to discuss singularity resolution. For completeness, let us first write out the four terms corresponding to $i, j = 1, 2$ (which are the most complicated of the 24 terms in $\hat{\mathcal{C}}_{\rm grav}$):

$$\begin{aligned}(\hat{\mathcal{C}}^{++}_{21}\Psi)(\lambda_1, \lambda_2, v) &= (v+2)\sqrt{v(v+4)}\\ &\quad\cdot\Psi\left(\frac{v+4}{v+2}\lambda_1, \frac{v+2}{v}\lambda_2, v+4\right),\end{aligned} \tag{3.31}$$

$$\begin{aligned}(\hat{\mathcal{C}}^{+-}_{21}\Psi)(\lambda_1, \lambda_2, v) &= v(v+2)\\ &\quad\cdot\Psi\left(\frac{v}{v+2}\lambda_1, \frac{v+2}{v}\lambda_2, v\right),\end{aligned} \tag{3.32}$$

$$\begin{aligned}(\hat{\mathcal{C}}^{-+}_{21}\Psi)(\lambda_1, \lambda_2, v) &= v(v-2)\\ &\quad\cdot\Psi\left(\frac{v}{v-2}\lambda_1, \frac{v-2}{v}\lambda_2, v\right),\end{aligned} \tag{3.33}$$

$$\begin{aligned}(\hat{\mathcal{C}}^{--}_{21}\Psi)(\lambda_1, \lambda_2, v) &= (v-2)\sqrt{v|v-4|}\\ &\quad\cdot\Psi\left(\frac{v-4}{v-2}\lambda_1, \frac{v-2}{v}\lambda_2, v-4\right).\end{aligned} \tag{3.34}$$

[4]Misner-like variables—volume and logarithms of metric components—were used in the brief discussion of Bianchi I models in [38]. This discussion already recognized that the use of volume as one of the arguments of the wave function would lead to simplifications. Dynamics was obtained by starting with the Hamiltonian constraint in the μ_o scheme from [35] and then substituting $\bar{\mu}_i$ of (3.9) for μ^i_o in the final result. This procedure does simplify the leading order quantum corrections to dynamics. In contrast, our goal is to simplify the full constraint. More importantly, constraint (3.20) is an improvement over that of [38] because we introduced $\bar{\mu}_i$ from the beginning of the quantization procedure and systematically defined the operators $\sin(\bar{\mu}_i c_i)$ (in Sec. III C).

Recall that, since v is proportional to the volume of the elementary cell, it vanishes when any one of the three directional scale factors a_i vanish. Thus, the classical singularity corresponds precisely to the points at which v vanishes. Now suppose that the function $\Psi(\lambda_1, \lambda_2, v)$ has no support on points $v = 0$ at an initial internal time T_o. As it evolves via (3.22), can it end up having support on such points? We will argue that this is impossible.

Let us decompose $\mathcal{H}^{\rm grav}_{\rm kin}$ as $\mathcal{H}^{\rm grav}_{\rm kin} = \mathcal{H}^{\rm grav}_{\rm sing} \oplus \mathcal{H}^{\rm grav}_{\rm reg}$, where $\Psi(\lambda_1, \lambda_2, v)$ is in $\mathcal{H}^{\rm grav}_{\rm sing}$ if it has support only on points with $v = 0$ and it is in $\mathcal{H}^{\rm grav}_{\rm reg}$ if it has no support on points with $v = 0$. Now, all the operators $\hat{\mathcal{C}}^{\pm\pm}_{ij}$ have a factor of $\sqrt{v}$ acting on the right [see Eq. (3.26)]. It ensures that each $\hat{\mathcal{C}}^{\pm\pm}_{ij}$ annihilates every state in $\mathcal{H}^{\rm grav}_{\rm sing}$. Therefore $\mathcal{H}^{\rm grav}_{\rm sing}$ is left invariant by the evolution. More importantly, because of the prefactors of $v \pm 2$ and $v \pm 4$ the action of the 4 operators in (3.31), (3.32), (3.33), and (3.34) preserves $\mathcal{H}^{\rm grav}_{\rm reg}$. This property is shared also by $\hat{\mathcal{C}}^{\pm\pm}_{ij}$ for other values of i, j and hence by $\hat{\mathcal{C}}_{\rm grav}$ and all its powers.[5] Therefore, the relational dynamics of (3.22) decouples $\mathcal{H}^{\rm grav}_{\rm sing}$ from $\mathcal{H}^{\rm grav}_{\rm reg}$. In particular, if one starts out with a "regular" quantum state at $T = 0$, it remains regular throughout the evolution. In this precise sense, the singularity is resolved.

Next, let us write out explicitly the full Hamiltonian constraint (3.22):

$$\partial_T^2 \Psi(\lambda_1, \lambda_2, v; T) = \frac{\pi G}{2}\sqrt{v}[(v+2)\sqrt{v+4}\Psi^+_4(\lambda_1, \lambda_2, v; T) - (v+2)\sqrt{v}\Psi^+_0(\lambda_1, \lambda_2, v; T) - (v-2)\sqrt{v}\Psi^-_0(\lambda_1, \lambda_2, v; T) + (v-2)\sqrt{|v-4|}\Psi^-_4(\lambda_1, \lambda_2, v; T)], \tag{3.35}$$

where $\Psi^\pm_{0,4}$ are defined as follows:

$$\Psi^\pm_4(\lambda_1, \lambda_2, v; T) = \Psi\Big(\frac{v \pm 4}{v \pm 2}\cdot\lambda_1, \frac{v \pm 2}{v}\cdot\lambda_2, v \pm 4; T\Big) + \Psi\Big(\frac{v \pm 4}{v \pm 2}\cdot\lambda_1, \lambda_2, v \pm 4; T\Big) + \Psi\Big(\frac{v \pm 2}{v}\cdot\lambda_1, \frac{v \pm 4}{v \pm 2}\cdot\lambda_2, v \pm 4; T\Big) + \Psi\Big(\frac{v \pm 2}{v}\cdot\lambda_1, \lambda_2, v \pm 4; T\Big) + \Psi\Big(\lambda_1, \frac{v \pm 2}{v}\cdot\lambda_2, v \pm 4; T\Big) + \Psi\Big(\lambda_1, \frac{v \pm 4}{v \pm 2}\cdot\lambda_2, v \pm 4; T\Big), \tag{3.36}$$

and

$$\Psi^\pm_0(\lambda_1, \lambda_2, v; T) = \Psi\Big(\frac{v \pm 2}{v}\cdot\lambda_1, \frac{v}{v \pm 2}\cdot\lambda_2, v; T\Big) + \Psi\Big(\frac{v \pm 2}{v}\cdot\lambda_1, \lambda_2, v; T\Big) + \Psi\Big(\frac{v}{v \pm 2}\cdot\lambda_1, \frac{v \pm 2}{v}\cdot\lambda_2, v; T\Big) + \Psi\Big(\frac{v}{v \pm 2}\cdot\lambda_1, \lambda_2, v; T\Big) + \Psi\Big(\lambda_1, \frac{v}{v \pm 2}\cdot\lambda_2, v; T\Big) + \Psi\Big(\lambda_1, \frac{v \pm 2}{v}\cdot\lambda_2, v; T\Big), \tag{3.37}$$

where, as before, we have given the restriction of the image of $\hat{\mathcal{C}}_{\rm grav}$ to the positive octant. Because $\mathcal{H}^{\rm grav}_{\rm reg}$ is left invariant by evolution we can in fact restrict λ_1, λ_2, and v to be strictly positive. On the right sides of (3.36) and (3.37), arguments of Ψ can take negative values. However, since $\Psi(\lambda_1, \lambda_2, v) = \Psi(|\lambda_1|, |\lambda_2|, |v|)$, we can just introduce absolute value signs on these arguments. Consequently, knowing the restriction of Ψ to the positive octant, (3.36) and (3.37) enable us to directly calculate its image under $\hat{\mathcal{C}}_{\rm grav}$. In particular, numerical evolutions can be carried out by restricting oneself to the positive octant.

Let us now examine the structure of this equation. As in the isotropic case, the right side is a difference equation. As far as the v dependence is concerned, the steps are uniform: the argument of the wave function involves $v - 4$, v, and $v + 4$ exactly as in the isotropic case. The step sizes are also the same as in [10] because, as noted above, our variable v is in precise agreement with that used in the isotropic case. There is again superselection. For each $\epsilon \in [0, 4)$, let us introduce a "lattice" $\mathcal{L}_\epsilon$ consisting of points $v = 4n$ if $\epsilon = 0$ and $v = 2n + \epsilon$ if $\epsilon \neq 0$.[6] Then the quantum evolution—as well as the action of the Dirac observables—preserves the subspaces $\mathcal{H}^\epsilon_{\rm phy}$ consisting of states with v support on $\mathcal{L}_\epsilon$. The most interesting of these sectors is the one labeled by $\epsilon = 0$ since it contains the classically singular points, $v = 0$. Therefore in what follows, unless otherwise stated, we will restrict ourselves to this sector.

The dependence of $\hat{\mathcal{C}}_{\rm grav}\Psi$ on λ_1, λ_2, by contrast, is much more difficult to control technically because the first two arguments of the wave function cannot be chosen to lie on a regular lattice in any simple way. In particular, even if

[5] To make this argument mathematically rigorous one would have to establish that $\hat{\mathcal{C}}_{\rm grav}$ is essentially self-adjoint and its self-adjoint extension also shares this property (or a suitable generalization thereof).

[6] As in the isotropic case, the lattice is doubled if $\epsilon \neq 0$ or 2 because of the symmetry property of our wave functions.

we started out with a wave function which has support only on a lattice, say $\lambda_1 = n\lambda_o$ for some λ_o, the action of $\hat{\mathcal{C}}_{\rm grav}$ shifts support to points such as $\lambda_1 = [(v \pm 2)/v]n\lambda_o$ which do not lie on this lattice. Thus, there is no obvious superselection with respect to λ_1 and λ_2; we have to work with the entire $\mathbb{R}^2$ they span. Had it been permissible to set $\bar{\mu}_i \propto /\sqrt{|p_i|}$, we could have restricted λ_i to lie on a regular lattice [36]. Then, following [40], we could have repeated the strategy used successfully in the isotropic case in [11] to simplify dynamics by carrying out a Fourier transform to pass to variables which are conjugate to λ_1, λ_2. However, as remarked earlier, that choice of $\bar{\mu}_i$ is inadmissible and hence the strategy cannot be repeated in the Bianchi I case. Nonetheless, it is still feasible to carry out numerical simulations. For, if one knows the support of the quantum state at an initial time T_o and the number of time steps across which one wants to evolve, one can calculate the number of points on a (irregular) grid in the λ_1-λ_2 plane on which the wave function will have support. Numerical work has in fact already commenced [41]. It would be interesting to investigate whether the efficient algorithms that have been introduced in the context of regular lattices [53] can be extended to this case.

We conclude this discussion by noting that it is possible to read off some qualitative features of dynamics from (3.35), (3.36), and (3.37). Since the steps in v of this difference equation are the same as those in the isotropic case, the dynamics of volume—and also of the matter density $\hat{\rho}_{\rm matt}$, since $\hat{p}_{(T)}$ is a constant of motion—would be qualitatively similar to that in the isotropic case. What about anisotropies? The λ_I ($I = 1, 2$) do not feature in the overall numerical factors in (3.35); they appear only in the argument of the wave functions. Under the action of $\hat{\mathcal{C}}_{\rm grav}$, these arguments get rescaled by factors $v \pm 4/v \pm 2$, $v \pm 2/v$, and $v/v \pm 2$. For large volumes, or more precisely low densities, these factors go as $1 + O(\rho_{\rm matt}/\rho_{\rm Pl})$. Hence, to leading order, we will recover the classical result that $a_1a_2a_3(H_i - H_j)$ are constants, where a_i are the directional scale factors and $H_i := d\ln a_i/dt$, the directional Hubble parameters. Since quantum corrections go as $\rho/\rho_{\rm Pl}$ they are utterly negligible away from the Planck regime.

In the next section we discuss three important features of dynamics dictated by (3.35) which provide significant physical intuition in complementary directions.

IV. PROPERTIES OF THE LQC QUANTUM DYNAMICS

This section is divided into three parts. Since we have used the same general procedure as in the isotropic case it is natural to ask how the quantum dynamics of (3.35) compares to that in [10]. In the first part we show that there is a natural projection from a dense subspace of the physical Hilbert space of the Bianchi I model to that of the Friedmann model which maps the Bianchi I Hamiltonian constraint to that of the Friedmann model. This result boosts confidence in the overall coherence and reliability of the quantization scheme used in LQC. In various isotropic models [10,14–16,18], one can derive certain effective equations. Somewhat surprisingly, for states which are semiclassical at a late initial time, they faithfully capture quantum dynamics throughout the entire evolution, including the bounce. The same considerations lead to effective equations in Bianchi I models which were already analyzed by Chiou and Vandersloot in Appendix C of [37]. In the second section we briefly discuss these equations and their consequences. In the third, we show that, as in the isotropic case [10,11], there is a precise sense in which the LQC quantum dynamics reduces to that of the Wheeler-DeWitt theory in the low curvature regime.

A. Relation to the LQC Friedmann dynamics

The problem of comparing dynamics of a more general system with that of a restricted, symmetry reduced one has been discussed in the literature in several contexts. In the classical theory, symmetric states often provide symplectic submanifolds $\Gamma_{\rm Res}$ of the more general phase spaces $\Gamma_{\rm Gen}$. Furthermore $\Gamma_{\rm Res}$ are preserved by the dynamics on $\Gamma_{\rm Gen}$. Therefore, it is tempting to repeat the same strategy in the quantum theory. Indeed, sometimes it is possible to find natural subspaces $\mathcal{H}_{\rm Res}$ of states with additional symmetry in the full Hilbert space $\mathcal{H}_{\rm Gen}$ of the more general system. However, generically $\mathcal{H}_{\rm Res}$ is not left invariant by the more general dynamics (see, e.g., [42,43]). In our case, one can introduce an isotropic subspace of $\mathcal{H}_{\rm Res}$ in the quantum theory based on any given fiducial cell $\mathcal{V}$: isotropic states correspond to wave functions $\Psi(\lambda_1, \lambda_2, v)$ which have support only at points $\lambda_1 = \lambda_2 = (v/2)^{1/3}$. (But note that this subspace is not invariantly defined; it is tied to $\mathcal{V}$.) It is easy to check that the space $\mathcal{H}_{\rm Res}$ of these states is not left invariant by the Bianchi I quantum dynamics (3.35).

However, this fact cannot be interpreted as saying that there is no simple relation between the quantum dynamics of the two theories: since restriction to $\mathcal{H}_{\rm Res}$ amounts to a sharp freezing of anisotropic degrees of freedom, in view of the quantum uncertainty principle, this procedure is not well suited to compare the quantum dynamics of the two systems. As pointed out in Sec. I, a better strategy is to integrate out the extra, anisotropic degrees of freedom. This would correspond to a *projection map* from $\mathcal{H}_{\rm Gen}$ to $\mathcal{H}_{\rm Res}$ rather than an embedding of $\mathcal{H}_{\rm Res}$ into $\mathcal{H}_{\rm Gen}$.

Consider first, as an elementary example, a particle moving in $\mathbb{R}^3$. Suppose that the potential depends only on z so that dynamics has a symmetry in the x, y directions. In the classical theory, there are several natural embeddings of the phase space $\Gamma_{\rm Res}$ into $\Gamma_{\rm Gen}$. For example, we can set $(z, p_z) \to (x = x_o, y = y_o, z; p_x = 0, p_y = 0, p_z)$ and the Hamiltonian vector field of the full theory is then

tangential to the images of each of these embeddings. However, in the quantum theory the Hilbert space $\mathcal{H}_{\rm Gen}$ of the full system is $L^2(\mathbb{R}^3, d^3x)$ and there is no natural embedding $\psi(z) \to \Psi(x, y, z)$. The classical strategy would suggest setting $\Psi(x, y, z) = \delta(x, x_o)\delta(y, y_o)\psi(z)$ but this is not a normalizable state in $\mathcal{H}_{\rm Gen}$ for any $\psi(z)$. Even if one were to ignore this fact and try to evolve these states, one would find that they are not preserved by the full Hamiltonian operator $\hat{H}$.

Note however that there *is* a natural projection $\hat{\mathbb{P}}$ from a dense subspace in $\mathcal{H}_{\rm Gen}$ to that in $\mathcal{H}_{\rm Res}$:

$$\Psi(x, y, z) \to (\hat{\mathbb{P}}\Psi)(z) := \int dx \int dy \Psi(x, y, z) \equiv \psi(z). \tag{4.1}$$

(For example, we can choose the dense subspace to be the space of smooth functions of compact support.) Furthermore, under this projection, the Hamiltonian operator

$$\hat{H} = -(\hbar^2/2m)\Delta + V(z)$$

of the general system is mapped to the Hamiltonian operator

$$\hat{h} := -(\hbar^2/2m)d^2/dz^2 + V(z)$$

of the reduced system. Hence solutions $\Psi(\vec{x}, t)$ of the Schrödinger equation of the full system are mapped to solutions $\psi(z, t)$ of the reduced system. Finally, this projection strategy continues to work for more general Hamiltonians of the type $f^i(z)p_i + V(z)$ which again have a symmetry in the x, y directions.

Let us return to the Bianchi I model and define a projection $\hat{\mathbb{P}}$ from states $\Psi(\lambda_1, \lambda_2, v)$ of the Bianchi I model to the states $\psi(v)$ of the Friedmann model of [10] as follows:

$$\Psi(\lambda_1, \lambda_2, v) \to (\hat{\mathbb{P}}\Psi)(v) := \sum_{\lambda_1, \lambda_2} \Psi(\lambda_1, \lambda_2, v) \equiv \psi(v). \tag{4.2}$$

(The idea of using such a map already appeared in [44] where the map was defined between elements of Cyl* of the locally rotationally symmetric Bianchi I model and that of the Friedmann model.) Again, $\hat{\mathbb{P}}$ is a well-defined projection from a dense subspace of the Bianchi I Hilbert space to a dense subspace of the Friedmann Hilbert space, consisting, for example, of states which have support only on a finite number of points. As is manifest from (4.2), its effect is to focus on volume by integrating out the anisotropic degrees of freedom with the same volume. Applying this projection map $\hat{\mathbb{P}}$ to Eq. (3.35), we find

$$\begin{aligned}\partial_T^2\psi(v;T) = 3\pi G[&(v+2)\sqrt{v(v+4)}\psi(v+4;T) \\ &- 2v^2\psi(v;T) + (v-2)\sqrt{v(v-4)} \\ &\times \psi(v-4;T)].\end{aligned} \tag{4.3}$$

This is *precisely* the quantum constraint describing the LQC dynamics of the Friedmann model with lapse[7] $N = |p|^{3/2}$. The reason for the exact agreement is twofold. First, the Hamiltonian constraint $\hat{\mathcal{C}}_{\rm grav}$ of the Bianchi I model is a difference operator whose coefficients depend *only* on v and, second, the shift in the argument is dictated *only* by v. Thus, conceptually, λ_1, λ_2 are "inert directions" in the same sense that x, y are in the elementary example discussed above. To summarize, there is a simple—and *exact*—relation between quantum dynamics of the two theories. It would be interesting to investigate if this result admits a suitable extension to other Bianchi models [33,54].

In completely general situations, of course, this exact agreement will not persist: the projected dynamics will provide extremely nontrivial corrections to the dynamics of the simpler system. However, the BKL conjecture says that the dynamics of general relativity greatly simplifies near spacelike singularities: In this regime, the time evolution at any one spatial point is well modeled by that of Bianchi I cosmology. Therefore, in a large class of situations there may well be a sense in which the quantum dynamics in the deep Planck regime can be projected to that of the Friedmann model with only small corrections. If so, the Planck scale quantum dynamics of the isotropic, homogeneous degree of freedom in the full theory will be much simpler than what one would have *a priori* expected.

B. Effective equations

Physically, the most interesting quantum states are those that are sharply peaked at a classical trajectory at late times. As explained in Sec. I, in the isotropic case such states remain peaked at certain effective trajectories at *all times*, including the epoch during which the Universe undergoes a quantum bounce. Thus, even in the deep Planck regime quantum physics is well captured by a smooth metric although its dynamics can no longer be approximated by the classical Einstein's equations and its components now contain large, $\hbar$-dependent terms. The effective equations obeyed by these geometries were first derived using ideas from geometrical quantum mechanics [55,56]. However, the assumptions made in these derivations break down in the deep Planck regime. Therefore *a priori* there was no reason to expect these equations to describe quantum dynamics so well also in the Planck regime. That they do was first shown by numerical simulations of the exact quantum equations [9,10] in the $k = 0$, $\Lambda = 0$ case. It was then realized that this model is in fact exactly soluble [11,57] and the power of the effective

[7] As noted at the end of Sec. III C, the analysis in [10] began with the lapse $N = 1$ and therefore leads to a slightly different factor ordering. Had one used $N = |p|^{3/2}$ from the beginning as in the current paper, one would have obtained the factor ordering used in [11]. Equation (4.3) matches exactly with that constraint.

equations could be attributed to this property. However, $k = 0$ models with *nonzero* cosmological constant and the closed $k = 1$ models do not appear to be exactly soluble. Yet, numerical solutions of the exact quantum equations show that the effective equations continue to capture full quantum dynamics extremely well [14–16].

New light was shed on this phenomenon by recent work on a path integral formulation of quantum cosmology [58]. The idea here is to return to the original derivation of path integrals due to Feynman and Hibbs [59] starting from quantum mechanics. In the isotropic case, then, the strategy is to *begin* with the kinematics and dynamics of LQC and then rewrite the transition amplitudes as path integrals. The resulting framework has several novel features. First, because the LQC kinematics relies on quantum geometry, paths that feature in the final integral are different from what one would have naively expected from the Wheeler-DeWitt theory. Second, the action that features in the measure is not the Einstein-Hilbert action but contains nontrivial quantum corrections. When expressed in the phase space language, $L = p\dot{q} - H(p, q)$, the ''Hamiltonian'' H turns out to be precisely the effective Hamiltonian constraint derived in [55,56], even though this casting of the LQC transition amplitudes in the path integral language is exact and does not presuppose that we are away from the Planck regime. Now, in the path integral approach, we have the following general paradigm. Consider the equations obtained by varying the action that appears in the path integral. (Generally these are just the classical equations but in LQC they turn out to be the effective equations of [10,16,56].) Fix a path representing a solution to these equations. If the action evaluated along this path is large compared to $\hbar$ then that solution is a good approximation to full quantum dynamics. If one applies this idea to isotropic LQC, one is led to conclude that solutions to the effective equations of [55,56] should be good approximations to full quantum dynamics also in the $k = 0$, $\Lambda \neq 0$, and $k = 1$ cases. This is precisely what one finds in numerical simulations. Thus, the path integral approach may well provide a deeper explanation of the power of effective equations. While such a path integral analysis is yet to be carried out in detail in the anisotropic case, because of the situation in the simpler cases it is of interest to find analogous effective equations and study their implications.

This task was carried out already by Chiou and Vandersloot in Appendix C of [37]. We will summarize the relevant results and briefly comment on the general picture that emerges.

Without loss of generality, we can restrict ourselves to the positive octant. Then the effective Hamiltonian constraint is given simply by the direct classical analog of (3.14):

$$\tfrac{1}{2}\, p_{(T)}^2 + \mathcal{C}_{\rm grav}^{\rm eff} = 0, \tag{4.4}$$

where

$$\mathcal{C}_{\rm grav}^{\rm eff} = -\frac{p_1 p_2 p_3}{8\pi G\gamma^2\Delta}[\sin\bar{\mu}_1 c_1 \sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_2 c_2 \sin\bar{\mu}_3 c_3 + \sin\bar{\mu}_3 c_3 \sin\bar{\mu}_1 c_1]. \tag{4.5}$$

Since $\sin x$ is bounded by 1 for all x, these equations immediately imply that the matter density, $\rho_{\rm matt} = p_{(T)}^2/2V^2 \equiv p_{(T)}^2/2p_1p_2p_3$, can never become greater than the critical density $\rho_{\rm crit} \approx 0.41\rho_{\rm Pl}$, first found in the isotropic case [10–12,16,18]. Since ρ becomes infinite at the big-bang singularity in the classical evolution, there is a precise sense in which the singularity is resolved in the effective theory.

Effective equations are obtained via Poisson brackets as in Sec. II but using (4.4) in place of the classical Hamiltonian constraint. This gives, for example,

$$\frac{dp_1}{d\tau} = \frac{p_1\sqrt{p_1p_2p_3}}{\sqrt{\Delta}\gamma\ell_{\rm Pl}} \cos(\bar{\mu}_1 c_1)(\sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_3 c_3), \tag{4.6}$$

and

$$\frac{dc_1}{d\tau} = -\frac{p_2p_3}{\Delta\gamma\ell_{\rm Pl}^2}\Big[\sin\bar{\mu}_1 c_1 \sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_1 c_1 \sin\bar{\mu}_3 c_3 + \sin\bar{\mu}_2 c_2 \sin\bar{\mu}_3 c_3 + \frac{\bar{\mu}_1 c_1}{2}\cos\bar{\mu}_1 c_1(\sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_3 c_3) - \frac{\bar{\mu}_2 c_2}{2}\cos\bar{\mu}_2 c_2(\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_3 c_3) - \frac{\bar{\mu}_3 c_3}{2}\cos\bar{\mu}_3 c_3(\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_2 c_2)\Big]. \tag{4.7}$$

Equations for p_2, c_2 and p_3, c_3 are obtained by cyclic permutations. These effective equations include ''leading order quantum corrections'' to the classical evolution equations (2.13) and (2.14). In any solution, these corrections become negligible in the distant past and in the distant future. As we noted in Sec. II, the shear Σ defined in Eq. (2.21) is a constant of motion in the classical theory. This is no longer the case in the effective theory. However, one can show that it remains finite throughout the evolution and becomes approximately constant in the low curvature region both in the distant past and in the distant future. Furthermore, its value in the distant future is the same as that in the distant past along any effective trajectory in the phase space.

Vandersloot (personal communication) has also carried out numerical integration of these equations. In the isotropic case each effective trajectory undergoes a quantum bounce when the matter density $\rho_{\rm matt}$ achieves a critical value $\rho_{\rm crit} \approx 0.41\rho_{\rm Pl}$. As one might expect, now the situation is more complicated because of the additional degrees of freedom. First, there are now several distinct ''bounces.'' More precisely, in addition to $\rho_{\rm matt}$ (or the

scalar curvature), we now have to keep track of the three Hubble rates H_i which directly control the Weyl curvature. In the backward evolution toward the classical big bang, Einstein's equations approximate the effective equations extremely well until the density of one of the H_i enters the Planck regime. Then the quantum corrections start rising quickly. Their net effect is to dilute the quantity in question. Once the quantity exits the Planck regime as a result of this dilution, quantum geometry effects again become negligible. Thus, as in the isotropic case, one avoids the ultraviolet-infrared tension [21] because the quantum geometry effects are extremely strong in the Planck regime but die off extremely quickly as the system exits this regime. Secondly, the volume or the density bounce occurs when the matter density is lower than $\rho_{\rm crit}$. This is not surprising because what matters is the total energy density and now there is also a contribution from gravitational waves. Finally, although there are distinct bounces for density (or scalar curvature) and the H_i (or the Weyl curvature invariants), they all occur near each other in the relational time T.

There are indications that the general scenario provided by effective equations captures the qualitative features of the full quantum evolution. However, the arguments are not conclusive. For conclusive evidence for (or against) this picture, one needs numerical simulations [41] of the exact quantum equations of Sec. III D, or a detailed, path integral treatment of the Bianchi I models along the lines of [58].

C. Relation to the Wheeler-DeWitt dynamics

Quantum dynamics of LQC is governed by a *difference*—rather than a *differential*—equation because of the quantum geometry effects. However, we will now show that, as in the isotropic case [10,11,16], the LQC quantum dynamics is well approximated by the WDW differential equation away from the Planck regime where quantum geometry effects become negligible.

In the WDW theory the directional scale factors and hence the three λ_i can assume any real value and it is simpler to work with the three λ_i rather than with λ_1, λ_2, and $v = 2\lambda_1\lambda_2\lambda_3$. Let us therefore set $\underline{\Psi}(\lambda_1, \lambda_2, \lambda_3; T) = \Psi(\lambda_1, \lambda_2, v; T)$ and assume that $\underline{\Psi}$ admits a smooth extension to all real values of λ_i. The idea is to pair various terms in Eqs. (3.36) and (3.37) in such a way so that two of the three arguments of $\underline{\Psi}$ are the same. For example, one such pair is

$$\underline{\Psi}\left(\frac{v+4}{v+2}\cdot\lambda_1, \frac{v+2}{v}\cdot\lambda_2, \lambda_3; T\right) \quad \text{and} \quad \underline{\Psi}\left(\frac{v}{v+2}\cdot\lambda_1, \frac{v+2}{v}\cdot\lambda_2, \lambda_3; T\right). \tag{4.8}$$

Next, let us define $v' = v + 2$ and $\lambda_2' = v'\lambda_2/(v' - 2)$ so that we have

$$\sqrt{v+4} = \sqrt{v'+2} = \sqrt{\left(\lambda_1 + \frac{1}{\lambda_2'\lambda_3}\right)\lambda_2'\lambda_3}. \tag{4.9}$$

Ignoring the common prefactors in Eqs. (3.36) and (3.37), the two paired terms in Eq. (4.8) can be expressed as

$$\begin{aligned}
&\sqrt{v'+2}\,\underline{\Psi}\left(\lambda_1 + \frac{1}{\lambda_2'\lambda_3}, \lambda_2', \lambda_3; T\right) - \sqrt{v'-2}\,\underline{\Psi}\left(\lambda_1 - \frac{1}{\lambda_2'\lambda_3}, \lambda_2', \lambda_3; T\right) \\
&\quad = \frac{2}{\lambda_2'\lambda_3}\frac{\partial}{\partial\lambda_1}\sqrt{v'}\underline{\Psi}(\lambda_1, \lambda_2', \lambda_3; T) + O\left(\left(\frac{1}{\lambda_2'\lambda_3}\right)^n \frac{\partial^n}{\partial\lambda_1^n}\sqrt{v'}\underline{\Psi}\right) \\
&\quad = \frac{4\lambda_1}{v'}\frac{\partial}{\partial\lambda_1}\sqrt{v'}\underline{\Psi}(\lambda_1, \lambda_2', \lambda_3; T) + O\left(\left(\frac{1}{\lambda_2'\lambda_3}\right)^n \frac{\partial}{\partial\lambda_1^n}\sqrt{v'}\underline{\Psi}\right),
\end{aligned} \tag{4.10}$$

where $n > 1$. [Notice that the v' in the denominator in front of the partial derivative will cancel the $v + 2$ prefactor in Eq. (3.35).] One can suitably pair all terms in (3.36) and (3.37) and express them as differential operators with corrections which are small for large values of λ_i. Let us ignore these corrections—i.e., assume that the $(1/\lambda_i\lambda_j)^n\partial_k^n\sqrt{v}\underline{\Psi}$ is negligible for $n > 1$ because $\underline{\Psi}$ is slowly varying and we are in the low density, large scale-factor regime. Then we find that the LQC Hamiltonian constraint (3.35) reduces to a rather simple differential equation:

$$\begin{aligned}
\partial_T^2\underline{\Psi}(\lambda_1, \lambda_2, \lambda_3; T) = \frac{8\pi G}{\sqrt{v}}\Bigg[&\lambda_1\frac{\partial}{\partial\lambda_1}\lambda_2\frac{\partial}{\partial\lambda_2} + \lambda_1\frac{\partial}{\partial\lambda_1}\lambda_3\frac{\partial}{\partial\lambda_3} + \lambda_2\frac{\partial}{\partial\lambda_2}\lambda_1\frac{\partial}{\partial\lambda_1} + \lambda_2\frac{\partial}{\partial\lambda_2}\lambda_3\frac{\partial}{\partial\lambda_3} + \lambda_3\frac{\partial}{\partial\lambda_3}\lambda_1\frac{\partial}{\partial\lambda_1} \\
&+ \lambda_3\frac{\partial}{\partial\lambda_3}\lambda_2\frac{\partial}{\partial\lambda_2}\Bigg](\sqrt{v}\underline{\Psi}(\lambda_1, \lambda_2, \lambda_3; T)).
\end{aligned} \tag{4.11}$$

This equation can be further simplified by introducing $\sigma_i = \log\lambda_i$ and $\underline{\Phi} = \sqrt{v}\underline{\Psi}$. The result is

$$\partial_T^2\underline{\Phi}(\sigma_1, \sigma_2, \sigma_3; T) = 16\pi G\left[\frac{\partial^2}{\partial\sigma_1\partial\sigma_2} + \frac{\partial^2}{\partial\sigma_1\partial\sigma_3} + \frac{\partial^2}{\partial\sigma_2\partial\sigma_3}\right]\underline{\Phi}(\sigma_1, \sigma_2, \sigma_3; T), \tag{4.12}$$

where v is now given by $2\exp(\sum \sigma_i)$. This is precisely the equation we would have obtained if we had started from the classical Hamiltonian constraint, used the Schrödinger quantization and the "covariant factor ordering" of the constraint as in the WDW theory. Thus, the LQC Hamiltonian constraint reduces to the WDW equation under the assumption that $\underline{\Psi}$ is slowly varying in the sense that $(1/\lambda_i\lambda_j)^n \partial_k^n \sqrt{v}\underline{\Psi}$ can be neglected for $n > 1$ relative to the term for $n = 1$. Since $(\lambda_i\lambda_j)^2$ is essentially the area of the i-j face of the fiducial cell $\mathcal{V}$ in Planck units, this should be an excellent approximation well away from the Planck regime. However, in the Planck regime itself the terms which are neglected in the LQC dynamics are comparable to the terms which are kept whence, as in the isotropic case, the WDW evolution completely fails to approximate the LQC dynamics.

V. DISCUSSION

In this paper we extended the improved LQC dynamics of Friedmann space-times [10] to obtain a coherent quantum theory of Bianchi I models. As in the isotropic case, we restricted the matter source to be a massless scalar field since it serves as a viable relational time parameter (a la Leibniz) both in the classical and quantum theories. However, it is rather straightforward to accommodate additional matter fields in this framework.

To incorporate the Bianchi I model, we had to overcome several significant obstacles. First, using discrete symmetries we showed that to specify dynamics it suffices to focus just on the positive octant. This simplified our task considerably. Second, in Sec. III B we introduced a more precise correspondence between LQG and LQC and used it to fix the parameters $\bar{\mu}_i$ that determine the elementary plaquettes, holonomies around which define the curvature operator $\hat{F}_{ab}{}^{k}$. This procedure led us to the expressions $\bar{\mu}_1^2 = (|p_1|\Delta\ell_{\rm Pl}^2)/|p_2 p_3|$, etc. They reduce to the expression $\bar{\mu}^2 = (\Delta\ell_{\rm Pl}^2)/|p|$ of the isotropic models [10,16,18]. But even there, the current reasoning has the advantage that it uses only quantum geometry, avoiding reference to classical areas even in the intermediate steps. However, because of this rather complicated dependence of $\bar{\mu}_i$ on p_i, the task of defining operators $\sin\bar{\mu}_i c_i$ seems hopelessly difficult at first. Indeed, this was the key reason why the earlier treatments [36,37,40] took a shortcut and simply set $\bar{\mu}_i^2 = (\Delta\ell_{\rm Pl}^2)/|p_i|$ by appealing to the relation $\bar{\mu}^2 = (\Delta\ell_{\rm Pl}^2)/|p|$ in the isotropic case. With this choice, quantization of the Hamiltonian constraint became straightforward and the final Bianchi I quantum theory resembled three copies of that of the Friedmann model. However, this result had the physically unacceptable consequence that significant departures from general relativity could occur in tame situations. By a nontrivial extension of the geometrical reasoning used in the isotropic case, in Sec. III C we were able to define the operators $\sin\bar{\mu}_i c_i$ for our expressions of $\bar{\mu}_i$. However, the structure of the resulting Hamiltonian constraint turned out to be rather opaque. To simplify its form, in Sec. III D we introduced volume as one of the arguments of the wave functions. The action of the gravitational part of the Hamiltonian constraint then became transparent: it turned out to be a difference operator where the multiplicative coefficients depend only on volume and the change in the arguments of the wave functions also depends only on volume; individual anisotropies do not feature in the action of the operator [see (3.35), (3.36), and (3.37)]. This simplification enabled us to show that the sector $\mathcal{H}^{\rm grav}_{\rm reg}$ of quantum states which have no support on classically singular configurations is preserved by quantum dynamics. In this precise sense the big-bang singularity is resolved. Furthermore, this quantum dynamics is free from the physical drawbacks of the older scheme mentioned above.

In Sec. IV we explored three consequences of quantum dynamics in some detail. First, we showed that there is a projection map $\hat{\mathbb{P}}$: $\mathcal{H}_{\rm Gen} \to \mathcal{H}_{\rm Res}$ from the Hilbert space of the more general Bianchi I model to that of the more restricted Friedmann model which maps the Bianchi I quantum constraint exactly to the Friedmann quantum constraint. This is possible because, as noted above, it is just the volume—rather than the anisotropies—that govern the action of the Bianchi I quantum constraint. This result is of considerable interest because, in view of the BKL conjecture, it suggests that near generic spacelike singularities the LQC of Friedmann models may capture qualitative features of the *full,* LQG dynamics of the isotropic, homogeneous degree of freedom. In Sec. IV B we briefly recalled the effective equations of Chiou and Vandersloot (see Appendix C of [37]). These equations provide intuition for the rich structure of quantum bounces in the Bianchi I model. Their analysis suggests that classical general relativity is an excellent approximation away from the Planck regime. However, in the Planck regime quantum geometry effects rise steeply and forcefully counter the tendency of the classical equations to drive the matter density, the Ricci scalar, and Weyl invariants to infinity. (In particular, as in the isotropic case, the matter density is again bounded above by $\rho_{\rm crit} \approx 0.41\rho_{\rm Pl}$.) Thus the quantum geometry effects dilute these quantities and, once the quantity exits the Planck regime, classical general relativity again becomes an excellent approximation. In Sec. IV C we showed that, as in the isotropic case [10,11,16], there is a precise sense in which LQC dynamics is well approximated by that of the WDW theory once quantum geometry effects become negligible.

The rather complicated dependence of $\bar{\mu}_i$ on p_i is also necessary to remove a fundamental conceptual limitation of the older treatments of the Bianchi I model. Recall that, because we have homogeneity and the spatial topology is noncompact, we have to introduce a fiducial cell $\mathcal{V}$ to construct a Lagrangian or a Hamiltonian framework. Of course, the final physical results must be independent of

this choice. At first this seems like an innocuous requirement but it turns out to be rather powerful. We will now recall from [40] the argument that this condition is violated with the simpler choice $\bar{\mu}_i^2 = (\Delta\ell_{\rm Pl}^2)/|p_i|$ but respected by the more complicated choice we were led to from LQG.

For definiteness, let us fix a fiducial metric ${}^o q_{ab}$ and denote by L_i the lengths of the edges of the fiducial cell $\mathcal{V}$. Suppose we were to use a different cell $\mathcal{V}'$ whose edges have lengths $L_i' = \beta_i L_i$ (no summation over i). Since the basic canonical fields A_a^i and E_i^a are insensitive to the choice of the cell, Eq. (2.3) implies that the labels c_i and p_i we used to characterize them change to $c_1' = \beta_1 c_1$, $p_1' = \beta_2\beta_3 p_1$, etc. The gravitational part of the classical Hamiltonian constraint (2.12) is just rescaled by an overall factor $(\beta_1\beta_2\beta_3)^2$ and the inverse symplectic structure is rescaled by $(\beta_1\beta_2\beta_3)^{-1}$. Hence the Hamiltonian vector field is rescaled by $(\beta_1\beta_2\beta_3)$, exactly as it should because the lapse is rescaled by the same factor. Thus, as one would expect, the classical Hamiltonian flow is insensitive to the change $\mathcal{V} \to \mathcal{V}'$. What is the situation in the quantum theory? Physical states belong to the kernel of the Hamiltonian constraint operator $\hat{C}_H$ whence the two quantum theories will carry the same physics only if $\hat{C}_H$ is changed at most by an overall rescaling. Analysis is a bit more involved than in the classical case because $\hat{C}_{\rm grav}$ involves factors of $\sin\bar{\mu}_i c_i$. Now, under $\mathcal{V} \to \mathcal{V}'$, our $\bar{\mu}_i$ transform as $\bar{\mu}_1 \to \bar{\mu}_1' = \beta_1^{-1}\bar{\mu}_1$, whence $\bar{\mu}_1' c_1' = \bar{\mu}_1 c_1$, etc., and the Hamiltonian constraint (3.14) is rescaled by an overall multiplicative factor $(\beta_1\beta_2\beta_3)^2$ just as in the classical theory. What happens if we set $\bar{\mu}_i^2 = \Delta\ell_{\rm Pl}^2/|p_i|$ as in [36,37,40]? Then, we are led to $\bar{\mu}_1' c_1' = (\beta_1/\sqrt{\beta_2\beta_3})\bar{\mu}_1 c_1$ etc. Since the constraint (3.14) is a sum of terms of the type $p_1 p_2 |p_3| \sin\bar{\mu}_1 c_1 \sin\bar{\mu}_2 c_2$ it has a rather uncontrolled transformation property and is not simply rescaled by an overall factor. It is then not surprising that, in the Planck regime, the dynamical predictions of the resulting quantum theory (as well as of the effective theory) depend on the choice of the elementary cell. It is rather remarkable that the more complicated form of $\bar{\mu}_i$ that we are led to from LQG kinematics has exactly the right form to make quantum dynamics insensitive to the choice of the fiducial cell $\mathcal{V}$. As mentioned above, it also ensures that the predictions of quantum theory are free of drawbacks of the earlier treatments [36], such as the correlation between the bounce and directional densities which do not have an invariant significance.

From physical considerations, as in the isotropic case, it would be most interesting to start at a "late time" with states that are sharply peaked at a classical solution in which the three scale factors assume values for which the curvature is tame and $p_{(T)}$ is very large compared to $\hbar$ in classical units $c = G = 1$. One would then evolve these states backward and forward in the internal time T. As we just discussed, analytical considerations show that, since the initial wave function is in $\mathcal{H}_{\rm reg}^{\rm grav}$, it will continue to be in that subspace; there is no danger that the expectation values of curvature, anisotropies, or density would diverge. But several important questions remain. Are there quantum bounces with a pre-big-bang branch again corresponding to a large, classical universe in the distant past? Is there a clear distinction between evolutions of data in which there are significant initial anisotropies and data which represent only perturbations on isotropic situations? Even in the second case, do anisotropies grow (or decay) following predictions of the classical theory or are there noticeable deviations because of accumulations of quantum effects over large time periods? Numerical simulations of the LQC equations are essential to provide confidence in (or rule out) the general scenario suggested by effective equations and to supply us with detailed Planck scale physics.

Finally, let us return to full LQG. At the present stage of development, there appears to be considerable freedom in the definition of the quantum Hamiltonian constraint in the full theory. Furthermore, our current understanding of the *physical implications* of these choices is quite limited. Already in the isotropic models, the improved dynamics scheme provided some useful lessons: it brought out the fact that these choices can be nontrivially narrowed down by carefully analyzing conceptual issues (e.g., requiring that the physical results should be independent of auxiliary structures introduced in the intermediate steps) and by working out the physical consequences of the theory in detail (to ensure that the quantum geometry effects are not dominant in the low energy regime). Rather innocuous choices—such as those made in arriving at the older μ_o scheme—can lead to unacceptable consequences on both these fronts [12]. The Bianchi I analysis has sharpened these lessons considerably. The fact that the kinematical interplay between LQG and LQC has a deep impact on the viability of quantum dynamics is especially revealing. A quantum analysis of inhomogeneous perturbations around Bianchi I backgrounds is therefore a promising direction for understanding the physical implications of the choices that have to be made in the definition of the Hamiltonian constraint in full LQG. Such an analysis is likely to narrow down choices and lead us to viable quantization schemes in LQG that lead to a good semiclassical behavior.

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APPENDIX: PARITY SYMMETRIES

In this Appendix we recall and extend results on parity symmetries obtained in [46].

In nongravitational physics, parity transformations are normally taken to be discrete diffeomorphisms $x_i \to -x_i$ in the physical space which are isometries of the flat 3-metric thereon. In the phase space formulation of general relativity, we do not have a flat metric—or indeed, any fixed metric. However, if the dynamical variables have internal indices—such as the triads and connections used in LQG—we can use the fact that the internal space I is a vector space equipped with a flat metric q_{ij} to define parity operations on the internal indices. Associated with any unit *internal* vector ξ^I, there is a parity operator Π_ξ which reflects the internal vectors in the 2-plane orthogonal to ξ. This operation induces a natural action on triads e^a_i, the connections A^i_a, and the conjugate momenta $P^a_i =: (1/8\pi G\gamma)E^a_i$ (since they are internal vectors or covectors). It turns out that e^a_i are proper internal covectors while A^i_a and P^a_i are pseudo-internal vectors and covectors, respectively. These geometrical considerations show that the Barbero-Immirzi parameter γ must change sign under any one of these parity operations, i.e., if it has the value $|\gamma|$ for, say, positively oriented triads, it should have the value $-|\gamma|$ for negatively oriented triads. Its value on degenerate triads is ambiguous, whence on the degenerate sector we cannot unambiguously recover the triads e^a_i from the momenta P^a_i. If one were to make γ a dynamical field [60–62], it follows that the field should be a *pseudoscalar* under internal parity transformations; geometrical considerations involving torsion have led to the same conclusion in [62]. (For details, see [63].)

In the diagonal Bianchi I model, we can restrict ourselves just to three parity operations Π_i. Under their action, the canonical variables c_i, p_i transform as follows:

$$\begin{aligned}\Pi_1(c_1, c_2, c_3) &= (c_1, -c_2, -c_3),\\ \Pi_1(p_1, p_2, p_3) &= (-p_1, p_2, p_3),\end{aligned} \tag{A1}$$

and the action of Π_2, Π_3 is given by cyclic permutations. Under any of these maps Π_i, the Hamiltonian (2.12) is left invariant. This is just as one would expect because Π_i are simply large gauge transformations of the theory under which the physical metric q_{ab} and the extrinsic curvature K_{ab} do not change. It is clear from the action (A1) that if one knows the dynamical trajectories on the octant $p_i \geq 0$ of the phase space, then dynamical trajectories on any other octant can be obtained just by applying a suitable (combination of) Π_i. Therefore, in the classical theory one can restrict one's attention just to the positive octant.

Let us turn to the quantum theory. We now have three operators $\hat{\Pi}_i$. Their action on states is given by

$$\hat{\Pi}_1 \Psi(\lambda_1, \lambda_2, \lambda_3) = \Psi(-\lambda_1, \lambda_2\lambda_3), \tag{A2}$$

etc. What is the induced action on operators? Since

$$\begin{aligned}\hat{\Pi}_1 \lambda_1 \hat{\Pi}_1 \Psi(\lambda_1, \lambda_2, \lambda_3) &= \hat{\Pi}_1(\lambda_1 \Psi(-\lambda_1, \lambda_2, \lambda_3))\\ &= -\lambda_1 \Psi(\lambda_1, \lambda_2, \lambda_3),\end{aligned} \tag{A3}$$

we have

$$\hat{\Pi}_1 \lambda_1 \hat{\Pi}_1 = -\lambda_1. \tag{A4}$$

The Hamiltonian constraint operator is given by Eqs. (3.20) and (3.21). To calculate its transformation property under parity maps, in addition to (A4), we also need the transformation property of operators $\sin\bar{\mu}_i c_i$. An inspection of Eq. (3.21) shows that, in view of the Bianchi I symmetries, it is sufficient to calculate $\hat{\Pi}_i \sin\bar{\mu}_1 c_1 \hat{\Pi}_i$. We have

$$\begin{aligned}\hat{\Pi}_1 \sin\bar{\mu}_1 c_1 \hat{\Pi}_1 \Psi(\lambda_1, \lambda_2, \lambda_3) &= \frac{1}{2i}\hat{\Pi}_1\left[\Psi\left(-\lambda_1 - \frac{\mathrm{sgn}(-\lambda_1)}{\lambda_2\lambda_3}, \lambda_2, \lambda_3\right) - \Psi\left(-\lambda_1 + \frac{\mathrm{sgn}(-\lambda_1)}{\lambda_2\lambda_3}, \lambda_2, \lambda_3\right)\right]\\ &= \frac{1}{2i}\left[\Psi\left(\lambda_1 - \frac{\mathrm{sgn}(\lambda_1)}{\lambda_2\lambda_3}, \lambda_2, \lambda_3\right) - \Psi\left(\lambda_1 + \frac{\mathrm{sgn}(\lambda_1)}{\lambda_2\lambda_3}, \lambda_2, \lambda_3\right)\right] = \sin\bar{\mu}_1 c_1 \Psi(\lambda_1, \lambda_2, \lambda_3),\end{aligned} \tag{A5}$$

whence

$$\hat{\Pi}_1 \sin\bar{\mu}_1 c_1 \hat{\Pi}_1 = \sin\bar{\mu}_1 c_1. \tag{A6}$$

An identical calculation shows that

$$\begin{aligned}\hat{\Pi}_2 \sin\bar{\mu}_1 c_1 \hat{\Pi}_2 \Psi(\lambda_1, \lambda_2, \lambda_3) &= \frac{1}{2i}\hat{\Pi}_2\left[\Psi\left(\lambda_1 - \frac{\mathrm{sgn}(\lambda_1)}{(-\lambda_2)\lambda_3}, -\lambda_2, \lambda_3\right) - \Psi\left(\lambda_1 + \frac{\mathrm{sgn}(\lambda_1)}{(-\lambda_2)\lambda_3}, -\lambda_2, \lambda_3\right)\right]\\ &= \frac{1}{2i}\left[\Psi\left(\lambda_1 + \frac{\mathrm{sgn}(\lambda_1)}{\lambda_2\lambda_3}, \lambda_2, \lambda_3\right) - \Psi\left(\lambda_1 - \frac{\mathrm{sgn}(\lambda_1)}{\lambda_2\lambda_3}, \lambda_2, \lambda_3\right)\right] = -\sin\bar{\mu}_1 c_1 \Psi(\lambda_1, \lambda_2, \lambda_3),\end{aligned} \tag{A7}$$

and similarly for $\hat{\Pi}_3$. Therefore, we have

$$\hat{\Pi}_2 \sin\bar{\mu}_1 c_1 \hat{\Pi}_2 = -\sin\bar{\mu}_1 c_1, \quad \text{and}$$
$$\hat{\Pi}_3 \sin\bar{\mu}_1 c_1 \hat{\Pi}_3 = -\sin\bar{\mu}_1 c_1. \tag{A8}$$

These transformation properties of $\sin\bar{\mu}_1 c_1$ under $\hat{\Pi}_i$ simply mirror the transformation properties of c_1 under the three parity operations Π_i in the classical theory. [Note that, because of the absolute value signs in the expressions (3.9), $\bar{\mu}_i$ do not change under any of the parity maps.]

From Eqs. (3.20) and (3.21) it now immediately follows that the gravitational part of the Hamiltonian constraint is left invariant under $\hat{\Pi}_i$. Since $\hat{p}^2_{(T)}$ is manifestly invariant, we have

$$\hat{\Pi}_i \hat{\mathcal{C}}_H \hat{\Pi}_i = \hat{\mathcal{C}}_H \tag{A9}$$

just as in the classical theory. Because of this invariance property, given any state $\Psi \in \mathcal{H}^{\text{grav}}_{\text{kin}}$, the restriction to the positive octant of its image under $\hat{\mathcal{C}}_{\text{grav}}$ determines its image everywhere on $\mathcal{H}^{\text{grav}}_{\text{kin}}$. As we saw in Sec. III D, this property simplifies the task of finding the explicit action of the Hamiltonian constraint considerably.

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