Loop quantum cosmology of Bianchi type II models

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The “improved dynamics” of loop quantum cosmology is extended to include the Bianchi type II model. Because these space-times admit both anisotropies and non-zero spatial curvature, certain technical difficulties arise over and above those encountered in the analysis of the (anisotropic but spatially flat) Bianchi type I space-times, and of the (spatially curved but isotropic) \( k=\pm 1 \) models. We address these and show that the big-bang singularity is resolved in the same precise sense as in the recent analysis of the Bianchi I model. Bianchi II space-times are of special interest to quantum cosmology because of the expected behavior of the gravitational field near generic space-like singularities in classical general relativity.

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I. INTRODUCTION

In this paper, we will study the loop quantum cosmology (LQC)\[1,2\] of the Bianchi type II model. These models are of special interest to the issue of singularity resolution because of the intuition derived from the body of results related to the Belinski, Khalatnikov, Lifshitz (BKL) conjecture\,[3,4] on the nature of generic, spacelike singularities in general relativity (see, e.g., [5]). Specifically, as the system enters the Planck regime, dynamics at any fixed spatial point is expected to be well described by the Bianchi I evolution. However, there are transitions in which the parameters characterizing the specific Bianchi I space-time change and the dynamics of these transitions mimics the Bianchi II time evolution. In a recent paper \[6\], we studied the Bianchi I model in the context of LQC. In this paper we will extend that analysis to the Bianchi II model. We will follow the same general approach and use the same notation, emphasizing only those points at which the present analysis differs from that of \[6\].

Bianchi I and II models are special cases of type A Bianchi models which were analyzed already in the early days of LQC (see in particular \[7,8\]). However, as is often the case with pioneering early works, these papers overlooked some important conceptual and technical issues. At the classical level, difficulties faced by the Hamiltonian (and Lagrangian) frameworks in non-compact, homogeneous space-times went unnoticed. In these cases, to avoid infinities, it is necessary to introduce an elementary cell and restrict all integrals to it \[9,10\]. The Hamiltonian frameworks in the early works did not carry out this step. Rather, they were constructed simply by dropping an infinite volume integral (a procedure that introduces subtle inconsistencies). In the quantum theory, the kinematical quantum states were assumed to be periodic —rather than almost-periodic— in the connection, and the
quantum Hamiltonian constraint was constructed using a “pre-$\mu_o$” scheme. Developments over the intervening years have shown that these strategies have severe limitations (see, e.g., [11, 12, 13, 14, 15]). In this paper, they will be overcome using ideas and techniques that have been introduced in the isotropic and Bianchi I models in these intervening years. Thus, as in [6] the classical Hamiltonian framework will be based on a fiducial cell, quantum kinematics will be constructed using almost periodic functions of connections and quantum dynamics will use the “$\bar{\mu}$ scheme.” Nonetheless, the space-time description of Bianchi II models in [7, 8], tailored to LQC, will provide the point of departure of our analysis.

New elements required in this extension from the Bianchi I model can be summarized as follows. Recall first that the spatially homogeneous slices $M$ in Bianchi models are isomorphic to 3-dimensional group manifolds. The Bianchi I group is the 3-dimensional group of translations. Hence the the three Killing vectors $^o\xi^a_i$ on $M$ — the left invariant vector fields on the group manifold — commute and coincide with the right invariant vector fields $^e\xi^a_i$ which constitute the fiducial orthonormal triads on $M$. In LQC one mimics the strategy used in LQG and spin foams and defines the curvature operator in terms of holonomies around plaquettes whose edges are tangential to these vector fields. The Bianchi II group, on the other hand, is generated by the two translations and the rotation on a null 2-plane. Now the Killing vectors $^o\xi^a_i$ no longer commute and neither do the fiducial triads $^e\xi^a_i$. Therefore we have to follow another strategy to build the elementary plaquettes. However, this situation was already encountered in the k=1, isotropic models [16, 17]. There, the desired plaquettes can be obtained by alternating between the integral curves of right and left invariant vector fields which do commute. However, in the isotropic case, the gravitational connection is given by $A^i_a = c^i \omega^a_i$, where $\omega^a_i$ are the covectors dual to $^e\xi^a_i$ and the holonomies around these plaquettes turned out to be almost periodic functions of the connection component $c^i$ [16, 17]. By contrast, in the Bianchi II model we have three connection components $c^i$ because of the presence of anisotropies, and, unfortunately, the holonomies around our plaquettes are no longer almost periodic functions of $c^i$. (This is also the case in more complicated Bianchi models.) Since the standard kinematical Hilbert space of LQC consists of almost periodic functions of $c^i$, these holonomy operators are not well-defined on this Hilbert space. Thus, the strategy [10] used so far in LQC to define the curvature operator is no longer viable.

One could simply enlarge the kinematical Hilbert space to accommodate the new holonomy functions of connections. But then the problem quickly becomes as complicated as full LQG. To solve the problem within the standard, symmetry reduced kinematical framework of LQC, one needs to generalize the strategy to define the curvature operator. Of course, the generalization must be such that, when applied to all previous models, it is compatible with the procedure of computing holonomies around suitable plaquettes used there. We will carry out this task by suitably modifying ideas that have already appeared in the literature. This generalization will enable one to incorporate all class A Bianchi models in the LQC framework.

Once this step is taken, one can readily construct the quantum Hamiltonian constraint and the physical Hilbert space, following steps that were introduced in the analysis [6] of the Bianchi I model. However, because Bianchi II space-times have spatial curvature, the spin connection compatible with the orthonormal triad is now non-trivial. It leads to two new terms in the Hamiltonian constraint that did not appear in the Bianchi I Hamiltonian. We will analyze these new terms in some detail. In spite of these differences, the big bang singularity is resolved in the same precise sense as in the Bianchi I model [6]: If a quantum
state is initially supported only on classically non-singular configurations, it continues to be supported on non-singular configurations throughout its evolution.

The paper is organized as follows. Section II summarizes the classical Hamiltonian theory describing Bianchi II models. Section III discusses the quantum theory. We first define a non-local connection operator $\hat{A}_a^i$ and use it to obtain the Hamiltonian constraint. We then show that the singularity is resolved and the Bianchi I quantum dynamics is recovered in the appropriate limit. In Section IV, we introduce effective equations for the model (with the same caveats as in the Bianchi I case [6]). Finally, in section V we summarize our results and discuss the new elements that appear in the Bianchi II model. In Appendix A we improve on the discussion of discrete symmetries presented in [6]. The results on the Bianchi I model obtained in [6] carry over without any change. But the change of viewpoint is important to the LQC treatment of the Bianchi II model and more general situations.

II. CLASSICAL THEORY

This section is divided into two parts. In the first we recall the structure of Bianchi II space-times and in the second we summarize the phase space formulation, adapted to LQC.

A. Diagonal Bianchi II Space-times

Because the issue of discrete symmetries is subtle in background independent contexts, and because it plays a conceptually important role in the quantum theory of Bianchi II models, we will begin with a brief summary of how various fields are defined [18, 19]. This stream-lined discussion brings out the assumptions which are often only implicit, making the discussion of discrete symmetries clearer.

In the Hamiltonian framework underlying loop quantum gravity (LQG), one fixes an oriented 3-manifold $M$ and a 3-dimensional ‘internal’ vector space $I$ equipped with a positive definite metric $q_{ij}$. The internal indices $i, j, k, \ldots$ are then freely lowered and raised by $q_{ij}$ and its inverse. A spatial triad $e^a_i$ is an isomorphism from $I$ to tangent space at each point of $M$ which associates a vector field $v^a := e^a_i v^i$ on $M$ to each vector $v^i$ in $I$. The dual co-triads are denoted by $\omega^a_i$. Given a triad, we acquire a positive definite metric $q_{ab} := q_{ij} \omega^i_a \omega^j_b$ on $M$. The metric $q_{ab}$ in turn singles out a 3-form $\epsilon^{abc}$ on $M$ which has positive orientation and satisfies $\epsilon^{abc} \epsilon^{def} q^{ad} q^{be} q^{cf} = 3!$. One can then define a 3-form $\epsilon_{ijk}$ on $I$ via $\epsilon_{ijk} = \epsilon_{abc} e^a_i e^b_j e^c_k$. Note that $\epsilon_{ijk}$ is automatically compatible with $q_{ij}$, i.e., $\epsilon_{ijk} \epsilon_{lmn} q^{il} q^{jm} q^{kn} = 3!$. If a triad $\tilde{e}^a_i$ is obtained by flipping an odd number of the vectors in the triad $e^a_i$, then $\tilde{e}^a_i$ and $e^a_i$ have opposite orientations and the fields they define satisfy $\tilde{q}_{ab} = q_{ab}$, $\tilde{\epsilon}_{abc} = \epsilon_{abc}$ but $\tilde{\epsilon}_{ijk} = -\epsilon_{ijk}$. Had we fixed $\epsilon_{ijk}$ once and for all on $I$, then $\epsilon_{abc}$ would have flipped sign under this operation and volume integrals on $M$ computed with the unbarred and barred triads would have had opposite signs. With our conventions, these volume integrals will not change and the parity flips will be symmetries of the symplectic structure and the Hamiltonian constraint.

The triad also determines an unique spin connection $\Gamma^a_i$ via

$$D_{[a} \omega^i_{b]} \equiv \partial_{[a} \omega^i_{b]} + \epsilon^j_{jk} \Gamma^j_{[a} \omega^k_{b]} = 0. \quad (2.1)$$

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1 Thus, in LQG one begins with non-degenerate triads and metrics, passes to the Hamiltonian framework and then, at the end, extends the framework to allow degenerate geometries.
The gravitational configuration variable $A^i_a$ is then given by $A^i_a = \Gamma^i_a + \gamma K^i_a$ where $K_{ab} := K^j_a \omega_{bj}$ is the extrinsic curvature of $M$ and $\gamma$ is the Barbero-Immirzi parameter, representing a quantization ambiguity. (The numerical value of $\gamma$ is fixed by the black hole entropy calculation.) The momenta $E^a_i$ carry, as usual, density weight 1 and are given by: $E^a_i = \sqrt{q} e^a_i$. The fundamental Poisson bracket is:

$$\{A^i_a(x), E^b_j(y)\} = 8\pi G \gamma \delta^a_i \delta^b_j \delta^3(x,y).$$  (2.2)

In Bianchi models \cite{20, 21, 22}, one restricts oneself to those phase space variables admitting a 3-dimensional group of symmetries which act simply and transitively on $M$. Thus, the 3-metrics $g_{ab}$ under consideration admit a 3-parameter group of isometries and $M$ is diffeomorphic to a 3-dimensional Lie group $G$. (However, there is no canonical diffeomorphism, so that there is no preferred point on $M$ corresponding to the identity element of $G$.) To avoid a proliferation of spaces and types of indices, it is convenient to identify the natural isomorphism between $LG \equiv I$ and Killing vector fields on $M$: for each internal vector $v^i$, $\xi^a_i v^i$ is a Killing field on $M$. For brevity we will refer to $\xi^a_i$ as (left invariant) vector fields on $M$. There is a canonical triad $\xi^1_i$ — the right invariant vector fields — which is Lie dragged by the $\xi^a_i$. This triad and the dual co-triad $\omega^i_a$ satisfy:

$$[\xi^a_i, \xi^b_j] = 0, \quad [\xi^a_i, \omega^b_j] = -C^b_{ik} \omega^k_j, \quad \omega^k_i = \frac{1}{2} C^b_{ik} \omega^b_j \wedge \omega^j_i,$$  (2.3)

where $C^b_{ik}$ denotes the structure constants of $LG$. It is convenient to use the fixed fields $\xi^a_i$ and $\omega^i_a$ as fiducial triads and co-triads.

In the case when $G$ is the Bianchi II group, we have $C^k_{ij} = 0$ as in all class A Bianchi models and, furthermore, the symmetric tensor $k^{ij} := C^k_{ij} \epsilon^{ijl}$ has signature $+,0,0$. Therefore, we can fix, once and for all an orthonormal basis $b^a_1, b^a_2, b^a_3$ in $I$ such that the only non-zero components of $C^k_{ij}$ are

$$C^1_{23} = -C^1_{32} = \tilde{\alpha},$$  (2.4)

where $\tilde{\alpha}$ is a non-zero real number.\footnote{Without loss of generality $\tilde{\alpha}$ can be chosen to be 1. We keep it general because we will rescale it later (see Eq. (2.17)) and because we want to be able to pass to the Bianchi I case by taking the limit $\tilde{\alpha} \to 0$.} We will assume that this basis is so oriented that

$$\epsilon_{123} := \epsilon_{ijk} b^a_1 b^a_2 b^a_3 = \varepsilon$$  (2.5)

where $\varepsilon = \pm 1$ depending on whether the frame $e^a_i$ (which determines the sign of $\epsilon_{ijk}$) is right or left handed. Throughout this paper we will set $\xi^a_i = \xi^a_i \alpha b^i_1, \xi^a_1 = \xi^a_i \alpha b^i_1, \omega^1_a = \omega^a_i \alpha b^i_1$, etc.

The form of the components of $C^k_{ij}$ in this basis implies that $M$ admits global coordinates $x, y, z$ such that the Bianchi II Killing vectors have the fixed form

$$\xi^1_i = \left( \frac{\partial}{\partial x} \right)^a, \quad \xi^2_i = \left( \frac{\partial}{\partial y} \right)^a, \quad \xi^3_i = \tilde{\alpha} y \left( \frac{\partial}{\partial x} \right)^a + \left( \frac{\partial}{\partial z} \right)^a.$$  (2.6)
These expressions bring out the fact that, if we were to attempt to compactify the spatial slices to pass to a $T^3$ topology—as one can in the Bianchi I model—we will no longer have globally well-defined Killing fields. Thus, in the Bianchi II model, we are forced to deal with the subtleties associated with non-compactness of the spatially homogeneous slices.

In the $x,y,z$ chart, the right invariant triad is given by

$$
\begin{align*}
\varrho_1^a &= \left( \frac{\partial}{\partial x} \right)^a, \\
\varrho_2^a &= \tilde{\alpha}z \left( \frac{\partial}{\partial x} \right)^a + \left( \frac{\partial}{\partial y} \right)^a, \\
\varrho_3^a &= \left( \frac{\partial}{\partial z} \right)^a,
\end{align*}
$$

and the dual co-triad by

$$
\omega_a^1 = (dx)_a - \tilde{\alpha}z(dy)_a, \\
\omega_a^2 = (dy)_a, \\
\omega_a^3 = (dz)_a.
$$

They determine a fiducial 3-metric $q_{ab} := q_{ij} \omega^i_a \omega^j_b$ with Bianchi II symmetries:

$$
q_{ab}dx^a dx^b = (dx - \tilde{\alpha}z dy)^2 + dy^2 + dz^2.
$$

In the diagonal models, the physical triads $e_i^a$ are related to the fiducial ones by

$$
\omega_a^i = a^i(\tau)\omega_a^i, \quad \text{and} \quad a_i(\tau)e_i^a = \varrho_i^a,
$$

where the $a_i$ are the three directional scale factors. Since the physical spatial metric is given by $q_{ab} = \omega_a^i \omega_b^i$, the space-time metric can be expressed as

$$
d\mathcal{S}^2 = -N d\tau^2 + a_1(\tau)^2(dx - \tilde{\alpha}z dy)^2 + a_2(\tau)^2 dy^2 + a_3(\tau)^2 dz^2
$$

where $N$ is the lapse function adapted to the time coordinate $\tau$.

For later use, let us calculate the spin connection (2.11) determined by triads $e_i^a$. From the definition of $\Gamma_a^i$ it follows that

$$
\Gamma_a^i = -\varepsilon^{ijk} e_j^b \left( \partial_a \omega_b j_k + \frac{1}{2} e_c^j \omega_a^i \partial_c \omega_b k \right).
$$

Using (2.3), the components of $\Gamma_a^i$ in the internal basis $^o\alpha_1^j, ~ ^o\alpha_2^j, ~ ^o\alpha_3^j$ can be expressed as

$$
\Gamma_a^1 = \frac{\tilde{\alpha} \varepsilon a_1^2}{2a_2 a_3} \omega_a^1; \quad \Gamma_a^2 = -\frac{\tilde{\alpha} \varepsilon a_2}{2a_3} \omega_a^2; \quad \Gamma_a^3 = -\frac{\tilde{\alpha} \varepsilon a_1}{2a_2} \omega_a^3.
$$

Before studying the dynamics of the model, let us examine the action of internal parity transformation $\Pi_\varepsilon$ which flips the $k$th triad vector and leaves the orthogonal vectors alone. (For details see Appendix and [19]). Under the parity transformation $\Pi_1$, for example, we have: $e_1^a \rightarrow -e_1^a, e_2^a \rightarrow e_2^a, e_3^a \rightarrow e_3^a$ and $a_1 \rightarrow -a_1, a_2 \rightarrow a_2, a_3 \rightarrow a_3$ whence $\Gamma_a^1 \rightarrow -\Gamma_a^1, \Gamma_a^2 \rightarrow \Gamma_a^2, \Gamma_a^3 \rightarrow -\Gamma_a^3$. Thus, both $e_i^a$ and $\Gamma_a^i$ are proper internal vectors. $\varepsilon$ on the other hand is a pseudo internal scalar, $\varepsilon \rightarrow -\varepsilon$ under every $\Pi_\varepsilon$. Note that the fiducial quantities carrying a label $o$ do not change under this transformation; it affects only the physical quantities.

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3 There is no sum if repeated indices are both covariant or contravariant. As usual, the Einstein summation convention holds if a covariant index is contracted with a contravariant index.
B. The Bianchi II Phase space

As is usual in LQC, we will now use the fiducial triads and co-triads to introduce a convenient parametrization of the phase space variables, $E_i^a, A_i^a$. Because we have restricted ourselves to the diagonal model and these fields are symmetric under the Bianchi II group, from each equivalence class of gauge related phase space variables we can choose a pair of the form

$$E_i^a = \tilde{p}_i \sqrt{|q|} \epsilon_i^a \quad \text{and} \quad A_i^a = \tilde{c}_i^a \omega_i^a, \quad (2.14)$$

where, as spelled out in footnote 3, there is no sum over $i$. Thus, a point in the phase space is now coordinatized by six real numbers $\tilde{p}_i, \tilde{c}_i^a$. One would now like to use the symplectic structure in full general relativity to induce a symplectic structure on our six-dimensional phase space. However, because of spatial homogeneity and the $R^3$ spatial topology, the integrals defining the symplectic structure, the Hamiltonian (and the action) all diverge. Therefore we have to introduce a fiducial cell $V$ and restrict integrals to it [9, 10]. We will take the fiducial cell to be rectangular with edges along the coordinate axes and lengths of $L_1, L_2$ and $L_3$ with respect to the fiducial metric $q_{ab}$. It then follows that the volume of the fiducial cell with respect to $q_{ab}$ is $V_o = L_1 L_2 L_3$. Then the non-zero Poisson brackets are given by:

$$\{\tilde{c}_i^a, \tilde{p}_j^b\} = \frac{8\pi G \gamma}{V_o} \delta_i^j \quad (2.15)$$

where $\gamma$ is the Barbero-Immirzi parameter. As in the Bianchi I case, we have a 1-parameter ambiguity in the symplectic structure because of the explicit dependence on $V_o$ and we have to make sure that the final physical results are either independent of $V_o$ or remain well-defined as we remove the ‘regulator’ and take the limit $V_o \to \infty$.

It is convenient to rescale variables to absorb this dependence in the phase space coordinates (as was done in the treatment of Bianchi I model in [6]). Let us set

$$p_1 = L_2 L_3 \tilde{p}_1, \quad p_2 = L_3 L_1 \tilde{p}_2, \quad p_3 = L_1 L_2 \tilde{p}_3, \quad (2.16)$$

$$c_1 = L_1 \tilde{c}_1, \quad c_2 = L_2 \tilde{c}_2, \quad c_3 = L_3 \tilde{c}_3 \quad \text{and} \quad \alpha = \frac{L_2 L_3}{L_1} \tilde{\alpha}, \quad (2.17)$$

where the last rescaling has been introduced to absorb factors of $L_i$ which would otherwise unnecessarily obscure the expression of the Hamiltonian constraint. The Poisson brackets between these new phase space coordinates is given by

$$\{\tilde{c}_i^a, p_j^b\} = 8\pi G \gamma \delta_i^j. \quad (2.18)$$

These variables have direct physical interpretation. For example, $p_1$ is the (oriented) area of the 2-3 face of the elementary cell with respect to the physical metric $q_{ab}$ and $h^{(1)} = \exp c_1 \tau_1$ is the holonomy of the physical connection $A_i^a$ along the first edge of the elementary cell.

Our choice (2.14) of physical triads and connections has fixed the internal gauge as well as the diffeomorphism freedom. Furthermore, it is easy to explicitly verify that, thanks to (2.14), the Gauss and the diffeomorphism constraints are automatically satisfied. Thus, as in [6], we are left just with the Hamiltonian constraint

$$C_H = \int_V \left[ \frac{N E_i^a E_b^b}{16 \pi G \sqrt{|q|}} (\epsilon_{ij} E_a^b - 2(1 + \gamma^2) K_{[a}^i K_{b]}^j) + N \mathcal{H}_{\text{matt}} \right] d^3x, \quad (2.19)$$
where

$$F_{ab}^k = 2\partial_{[a}A_{b]}^k + \epsilon_{ij}^k A_a^i A_b^j$$  \hspace{1cm} (2.20)

is the curvature of $A_a^i$ and $\mathcal{H}_{\text{matt}}$ is the matter Hamiltonian density. As in [6], our matter field will consist only of a massless scalar field $T$ which will later serve as a relational time variable a la Liebniz. (Additional matter fields can be incorporated in a straightforward manner, modulo possible intricacies of essential self-adjointness.) Thus,

$$\mathcal{H}_{\text{matt}} = \frac{1}{2} \frac{p_1^2}{\sqrt{|q|}}$$  \hspace{1cm} (2.21)

Since we want to use the massless scalar field as relational time, it is convenient to use a harmonic-time gauge, i.e., assume that the time coordinate $\tau$ in (2.11) satisfies $\Box \tau = 0$. The corresponding lapse function is $N = \sqrt{|p_1 p_2 p_3|}$. With this choice, the Hamiltonian constraint simplifies considerably. Note first that the basic canonical variables can be expanded as

$$E_i^a = \frac{p_i}{V_o} L_i \sqrt{|q|} \epsilon_i^a \quad \text{and} \quad A_i^a = \frac{c_i}{L_i} \omega_i^a,$$  \hspace{1cm} (2.22)

and the extrinsic curvature is given by

$$K_a^i = \gamma^{-1} (A_i^a - \Gamma_a^i).$$

Next, using $p_1 = (\text{sgn} a_1) |a_2 a_3| L_2 L_3$ etc, the components of the spin connection become:

$$\Gamma_a^1 = \frac{\alpha \varepsilon p_2 p_3 \omega_1^2}{2 p_1^2} \frac{L_2}{L_1}, \quad \Gamma_a^2 = -\frac{\alpha \varepsilon p_3 \omega_1^2}{2 p_1} \frac{L_2}{L_3}, \quad \Gamma_a^3 = -\frac{\alpha \varepsilon p_2 \omega_1^2}{2 p_1} \frac{L_2}{L_3}.$$  \hspace{1cm} (2.23)

Collecting terms, the Hamiltonian constraint (2.19) becomes

$$\mathcal{C}_H = -\frac{1}{8 \pi G \gamma^2} \left[ p_1 p_2 c_1 c_2 + p_2 p_3 c_2 c_3 + p_3 p_1 c_3 c_1 + \alpha \varepsilon p_2 p_3 c_1 \right.$$

$$\left. - (1 + \gamma^2) \left( \frac{\alpha p_2 p_3}{2 p_1} \right)^2 \right] + \frac{1}{2} p_T^2$$

$$= \mathcal{C}_H^{(\text{BI})} - \frac{1}{8 \pi G \gamma^2} \left[ \alpha \varepsilon p_2 p_3 c_1 - (1 + \gamma^2) \left( \frac{\alpha p_2 p_3}{2 p_1} \right)^2 \right].$$  \hspace{1cm} (2.24)

where $\mathcal{C}_H^{(\text{BI})}$ is the Hamiltonian constraint (including the matter term) for Bianchi I space-times which has already been studied in [6]. Note that this constraint is recovered in the limit $\alpha \rightarrow 0$, as it must be.

Knowing the form of the Hamiltonian constraint, it is now possible to derive the time evolution of any classical observable $\mathcal{O}$ by taking its Poisson bracket with $\mathcal{C}_H$:

$$\dot{\mathcal{O}} = \{ \mathcal{O}, \mathcal{C}_H \},$$  \hspace{1cm} (2.26)

where the ‘dot’ stands for derivative with respect to harmonic time $\tau$. This gives

$$\dot{p}_1 = \gamma^{-1} (p_1 p_2 c_2 + p_1 p_3 c_3 + \alpha \varepsilon p_2 p_3),$$  \hspace{1cm} (2.27)

$$\dot{p}_2 = \gamma^{-1} (p_2 p_1 c_1 + p_2 p_3 c_3).$$  \hspace{1cm} (2.28)
\[ \dot{p}_3 = \gamma^{-1}(p_3 p_1 c_1 + p_3 p_2 c_2), \quad (2.29) \]
\[ \dot{c}_1 = -\frac{1}{\gamma}(p_2 c_1 c_2 + p_3 c_1 c_3 + \frac{1}{2p_1}(1 + \gamma^2)(\frac{\alpha p_2 p_3}{p_1}), \quad (2.30) \]
\[ \dot{c}_2 = -\frac{1}{\gamma}(p_1 c_2 c_1 + p_3 c_2 c_3 + \alpha \varepsilon p_3 c_1 - \frac{1}{2p_2}(1 + \gamma^2)(\frac{\alpha p_2 p_3}{p_1}), \quad (2.31) \]
\[ \dot{c}_3 = -\frac{1}{\gamma}(p_1 c_3 c_1 + p_2 c_3 c_2 + \alpha \varepsilon p_2 c_1 - \frac{1}{2p_3}(1 + \gamma^2)(\frac{\alpha p_2 p_3}{p_1}). \quad (2.32) \]

Any initial data satisfying the Hamiltonian constraint can be evolved by using the six equations above. It is straightforward to extend these results if there are additional matter fields.

Finally, let us consider the parity transformation \( \Pi_k \) which flips the \( k \)th physical triad vector \( e^a_k \). (As noted before, this transformation does not act on any of the fiducial quantities which carry a label \( o \).) Under this map, we have: \( q_{ab} \to q_{ab}, \epsilon_{abc} \to \epsilon_{abc} \) but \( \epsilon_{ijk} \to -\epsilon_{ijk}, \varepsilon \to -\varepsilon \). The canonical variables \( c^i, p_i \) transform as proper internal vectors and co-vectors: For example

\[ \Pi_1(c_1, c_2, c_3) \to (-c_1, c_2, c_3) \quad \text{and} \quad \Pi_1(p_1, p_2, p_3) \to (-p_1, p_2, p_3). \quad (2.33) \]

Consequently, both the symplectic structure and the Hamiltonian constraint are left invariant under any of the parity maps \( \Pi_k \).

This Hamiltonian description will serve as the point of departure for loop quantization in the next section.

### III. QUANTUM THEORY

This section is divided into three parts. In the first, we discuss the kinematics of the model, in the second we define an operator corresponding to the connection \( A^i_a \), using holonomies and in the third we introduce the Hamiltonian constraint operator and describe its action on states.

#### A. LQC Kinematics

The kinematics for the LQC of Bianchi II models is almost identical to that for Bianchi I models. Therefore, in the sub-section we closely follow [6].

Let us begin by specifying the elementary functions on the classical phase space which will have unambiguous analogs in the quantum theory. As in the Bianchi I model, the elementary variables are the momenta \( p_i \) and holonomies of the gravitational connection \( A^i_a \) along the integral curves of the right invariant vector fields \( \varphi^a_i \). Let \( \tau_i \) be a basis of the Lie algebra of \( SU(2) \), satisfying \( \tau_i \tau_j = \frac{i}{2} \epsilon^k_{ij} \tau_k - \frac{1}{2} \delta_{ij} \mathbb{I} \) where \( \mathbb{I} \) is the unit \( 2 \times 2 \) matrix. Consider an edge of length \( \ell L_k \) with respect to the fiducial metric \( q_{ab} \), parallel to \( \varphi^a_k \). The holonomy \( h^\ell_k \) along it is given by

\[ h^\ell_k(c_1, c_2, c_3) = \exp(\ell c_k \tau_k) = \cos \frac{\ell c_k}{2} \mathbb{I} + 2 \sin \frac{\ell c_k}{2} \tau_k. \quad (3.1) \]
(Note that $\ell$ depends of the fiducial cell but not on the fiducial metric.) This family of holonomies is completely determined by the almost periodic functions $\exp(i\ell c_k)$ of the connection. These almost periodic functions will be our elementary configuration variables which will be promoted unambiguously to operators in the quantum theory.

It is simplest to use the $p$-representation to specify the gravitational sector $\mathcal{H}^{\text{grav}}_{\text{kin}}$ of the kinematic Hilbert space. The orthonormal basis states $|p_1, p_2, p_3\rangle$ are eigenstates of quantum geometry. For example, in the state $|p_1, p_2, p_3\rangle$ the face $S_{23}$ of the fiducial cell $V$ (given by $x = \text{const}$) has area $|p_1|$. The basis is orthonormal in the sense

$$
\langle p_1, p_2, p_3 | p_1', p_2', p_3' \rangle = \delta_{p_1 p_1'} \delta_{p_2 p_2'} \delta_{p_3 p_3'},
$$

where the right side features Kronecker symbols rather than the Dirac delta distributions. Hence kinematical states can consist only of countable linear combinations

$$
|\Psi\rangle = \sum_{p_1, p_2, p_3} \Psi(p_1, p_2, p_3) |p_1, p_2, p_3\rangle
$$

of these basis states for which the norm

$$
||\Psi||^2 = \sum_{p_1, p_2, p_3} |\Psi(p_1, p_2, p_3)|^2
$$

is finite. Because the right side features a sum over a countable number of points on $\mathbb{R}^3$, rather than a 3-dimensional integral, LQC kinematics are inequivalent to those of the Schrödinger approach used in Wheeler-DeWitt quantum cosmology.

Next, recall that on the classical phase space the three reflections $\Pi_i : e_i^a \rightarrow -e_i^a$ are large gauge transformations under which physics does not change (since both the metric and the extrinsic curvature are left invariant). These large gauge transformations have a natural induced action, denoted by $\hat{\Pi}_i$, on the space of wave functions $\Psi(p_1, p_2, p_3)$. For example,

$$
\hat{\Pi}_1 \Psi(p_1, p_2, p_3) = \Psi(-p_1, p_2, p_3).
$$

Since $\hat{\Pi}_i^2$ is the identity, for each $i$, the group of these large gauge transformations is simply $\mathbb{Z}_2$. As in Yang-Mills theory, physical states belong to its irreducible representation. For definiteness, as in the isotropic and Bianchi I models, we will work with the symmetric representation. It then follows that $\mathcal{H}^{\text{grav}}_{\text{kin}}$ is spanned by wave functions $\Psi(p_1, p_2, p_3)$ which satisfy

$$
\Psi(p_1, p_2, p_3) = \Psi(|p_1|, |p_2|, |p_3|)
$$

and have a finite norm (3.4).

The action of the elementary operators on $\mathcal{H}^{\text{grav}}_{\text{kin}}$ is as follows: the momenta act by multiplication whereas the almost periodic functions in $c_i$ shift the $i$th argument. For example,

$$
[\hat{p}_1 \Psi](p_1, p_2, p_3) = p_1 \Psi(p_1, p_2, p_3) \quad \text{and} \quad \left[ \exp(i\ell c_1) \Psi \right](p_1, p_2, p_3) = \Psi(p_1 - 8\pi\gamma G\ell, p_2, p_3).
$$

The expressions for $\hat{p}_2, \exp(i\ell c_2), \hat{p}_3$ and $\exp(i\ell c_3)$ are analogous. Finally, we need to define the operator $\hat{\varepsilon}$ since $\varepsilon$ features in the expression of the Hamiltonian constraint. In the classical theory, $\varepsilon$ is unambiguously defined on non-degenerate triads, i.e., when $p_1p_2p_3 \neq 0$. 


In quantum theory, wave functions can have support also on degenerate configurations. We will extend the definition to degenerate triads using the basis \( |p_1, p_2, p_3 \rangle \):

\[
\hat{\varepsilon} |p_1, p_2, p_3 \rangle := \begin{cases} 
|p_1, p_2, p_3 \rangle & \text{if } p_1p_2p_3 \geq 0, \\
-|p_1, p_2, p_3 \rangle & \text{if } p_1p_2p_3 < 0.
\end{cases} \tag{3.8}
\]

Finally, the full kinematical Hilbert space \( \mathcal{H}_{\text{kin}} \) will be the tensor product \( \mathcal{H}_{\text{kin}} = \mathcal{H}_{\text{kin}}^{\text{grav}} \otimes \mathcal{H}_{\text{kin}}^{\text{matt}} \), where \( \mathcal{H}_{\text{kin}}^{\text{matt}} = L^2(\mathbb{R}, dT) \) is the matter kinematical Hilbert space for the homogeneous scalar field. On \( \mathcal{H}_{\text{kin}}^{\text{matt}} \), \( \hat{T} \) will act by multiplication and \( \hat{p}_T := -i\hbar dT \) will act by differentiation. As in isotropic and Bianchi I models, our final results would remain unaffected if we use a “polymer representation” also for the scalar field.

**B. The connection operator \( \hat{A}_a^i \)**

To define the quantum Hamiltonian constraint, we cannot directly use the symmetry reduced classical constraint \( (2.24) \) because it contains connection components \( c_k \) themselves and in LQC only almost periodic functions of \( c_k \) have unambiguous operator analogs. Indeed, in all LQC models considered so far \([3, 10, 11, 16, 17, 23, 24, 25]\), we were led to return to the expression \( (2.19) \) in the full theory and mimic the procedure used in LQG \([26]\). More precisely, the key strategy was to follow full LQG (and spin foams) and define a “field strength operator” using holonomies around suitable closed loops. In the Bianchi I model, these closed loops were formed by following integral curves of right invariant vector fields (which are also left invariant). As mentioned in section \( \text{III} \) in the Bianchi II model the right invariant vector fields define the fiducial triads \( \gamma^a_i \), the left invariant vector fields, the Killing fields \( \xi^i \). Neither constitutes a commuting set, whence their integral curves cannot be used to form closed loops. However, as in the \( k=1 \) case \([16, 17]\), one can hope to exploit the fact that the right invariant vector fields do commute with the left invariant ones and construct the closed loops by alternately following right and left invariant vector fields. But, as mentioned in section \( \text{III} \) a new problem arises: unlike in the \( k=1 \) (or Bianchi I) model the resulting holonomies are no longer almost periodic functions of \( c_k \), whence the Hilbert space \( \mathcal{H}_{\text{kin}}^{\text{grav}} \) does not support these holonomy operators. For completeness we will first show this fact explicitly and then introduce a new avenue to bypass this difficulty.

The problematic curvature component turns out to be \( F_{yz}^{-1} \). To construct the corresponding operator, following the strategy used in the \( k=1 \) case \([16, 17]\), we will construct a closed loop \( \Box_{yz} \) as follows. In the coordinates \((x, y, z)\), i) Move from \((0, 0, 0)\) to \((0, \bar{\mu}_2 L_2, 0)\) following \( \xi^2_3 \); ii) then move from \((0, \bar{\mu}_2 L_2, 0)\) to \((0, \bar{\mu}_2 L_2, \bar{\mu}_3 L_3)\) following \( \gamma^3_2 \); iii) then move from \((0, \bar{\mu}_2 L_2, \bar{\mu}_3 L_3)\) to \((0, 0, \bar{\mu}_3 L_3)\) following \( -\xi^3_2 \); and, finally, iv) move from \((0, 0, \bar{\mu}_3 L_3)\) to \((0, 0, 0)\) following \( -\gamma^3_2 \). The parameters \( \bar{\mu}_2, \bar{\mu}_3 \) which determine the ‘lengths’ of these edges can be fixed by the semi-heuristic correspondence between LQC and LQG exactly as in the Bianchi I model \([6]\) because the geometric considerations used in that analysis continue to hold without any modification in all Bianchi models with \( \mathbb{R}^3 \) spatial topology:

\[
\bar{\mu}_1 = \sqrt{\frac{|p_1| \Delta \ell^2_{P_1}}{|p_2p_3|}}; \quad \bar{\mu}_2 = \sqrt{\frac{|p_2| \Delta \ell^2_{P_1}}{|p_1p_3|}}; \quad \bar{\mu}_3 = \sqrt{\frac{|p_3| \Delta \ell^2_{P_1}}{|p_1p_2|}} \tag{3.9}
\]

where \( \Delta \ell^2_{P_1} = 4\sqrt{3}\pi \gamma \ell^2_{P_1} \) is the ‘area gap’. The holonomy around this closed loop \( \Box_{yz} \) is
given by
\[ h_{\square_{yz}} = \frac{2}{c \bar{\mu}_2 \bar{\mu}_3 L_2 L_3} \cos \left( \frac{\bar{\mu}_2 c_2}{2} \right) \sin \left( \frac{\bar{\mu}_2 c_2}{2} \right) \left( c_2 \sin(\bar{\mu}_3 c_3) + \alpha \bar{\mu}_3 c_1 \cos(\bar{\mu}_3 c_3) \right) \] (3.10)

where
\[ c = \sqrt{\alpha^2 \bar{\mu}_2^2 c_2^2 + c_2^2}. \] (3.11)

If we were to shrink the loop so that the area it encloses goes to zero, we do indeed recover the classical expression of $F_{yz}$. However, because of presence of the term $c$, if $\alpha \neq 0$ the right side fails to be almost periodic in $c_1$ and $c_2$. Hence this holonomy operator fails to exist on $H_{\text{kin}}$. It is clear from the expression (3.11) of $c$ that the problem is independent of the specific way $\bar{\mu}_i$ are fixed.

We will bypass this difficulty by mimicking another strategy used in full LQG [26]: We will use holonomies along segments parallel to $\omega_a$ to define an operator corresponding to the connection itself. This is a natural strategy because holonomies along these segments suffice to separate the Bianchi II connections (2.14). Let us set $A_a := A_a^k \tau_k$. Then we have the identity:
\[ A_a = \lim_{\ell_k \to 0} \sum_k \frac{1}{2\ell_k L_k} \left( h_k^{(\ell_k)} - (h_k^{(\ell_k)})^{-1} \right) \] (3.12)

where $h_k^{(\ell_k)}$ is given by (3.1). In the expressions of physically interesting operators such as the Hamiltonian constraint of full LQG, one often replaces $A_a$ with the (analog of the) right side of (3.12). But because of the specific forms of these operators, the limit trivializes on diffeomorphism invariant states of LQG. In LQC, we have gauge fixed the system and therefore cannot appeal to diffeomorphism invariance. Indeed, while the holonomies are well-defined for each non-zero $\ell_k$, the limit fails to exist on $H_{\text{grav}}$. A natural strategy is to shrink $\ell_k$ to a judiciously chosen non-zero value. But what would this value be? In the case of plaquettes, we could use the interplay between LQG and LQC directly because the argument $p_i$ of LQC quantum states refers to quantum areas of faces of the elementary cell $V$. For edges we do not have such direct guidance. There is, nonetheless a natural principle one can adopt: Normalize $\ell_k$ such that the numerical coefficient in front of the curvature operator constructed from the resulting connection agrees with that in the expression of the curvature operator constructed from holonomies around closed loops, in all cases where the second construction is available. We will use this strategy. Let us apply it to the Bianchi I model where $F^k_{ab} = \epsilon_{ij}^k A^i_a A^j_b$. Using holonomies around closed loops one obtains the field strength operator
\[ \hat{F}^k_{ab} = \epsilon_{ij}^k \left( \frac{\sin \bar{\mu} c}{\bar{\mu} L} \omega^i_a \right) \left( \frac{\sin \bar{\mu} c}{\bar{\mu} L} \omega^j_b \right) \] (3.13)

where
\[ \left( \frac{\sin \bar{\mu} c}{\bar{\mu} L} \omega^i_a \right) = \left( \frac{\sin \bar{\mu} c_i}{\bar{\mu} L_i} \omega^i_a \right) \] (no sum over $i$)

(see Eqs (3.12) and (3.13) in [6]). Therefore, our strategy yields $\ell_k = 2\bar{\mu}_k$, that is,
\[ \hat{A}_a^k = \frac{\sin (\bar{\mu}_k c_k)}{\bar{\mu}_k L_k} \omega^k_a, \] (3.14)

where there is no sum over $k$. Note that the principle stated above leads us unambiguously to the factor 2 in $\ell_k = 2\bar{\mu}_k$; without recourse to a systematic strategy, one may have naively set $\ell_k = \bar{\mu}_k$. 


If we compare the expression (3.14) of the connection operator with the expression (2.14) of the classical connection, we have effectively defined an operator \( \hat{c} \) via

\[
\hat{c}_k = \frac{\sin(\bar{\mu}^k c_k)}{\bar{\mu}^k}
\]

(3.15)

where there is again no sum over \( k \). In the literature such a quantization of \( c \) is often called “polymerization.” Our approach is an improvement over such strategies in two respects. First, we did not just make the substitution \( c \rightarrow \sin \ell c / \ell \) by hand; a priori one could have used another substitution such as \( c \rightarrow \tan \ell c / \ell \). Rather, as in full LQG, we used the strategy of expressing the connection in terms of holonomies, ‘the elementary variables’. But this still leaves open the question of what \( \ell \) one should use. We determined this by requiring that the overall normalization of \( \hat{F}_{ab}^k \) constructed from \( \hat{A}_a^i = c^i (L^i)^{-1} a^i \) should agree with that of \( \hat{F}_{ab}^k \) constructed from holonomies around appropriate closed loops, when the second construction is possible. Therefore, our construction is a bona-fide generalization of the previous constructions used successfully in LQC.

This strategy has some applications beyond the Bianchi II model studied in this paper. First, the \( k = -1 \) isotropic case has been studied in detail in [23, 24]. The analysis uses the \( \bar{\mu} \) scheme, carries out a numerical simulation using exact LQC equations and shows that the effective equations of the “embedding approach” [27, 28] (discussed in section IV) provide an excellent approximation to the quantum evolution. While this is an essentially exhaustive treatment, as [23, 24] itself points out, the treatment has a conceptual limitation in that it builds holonomies around the closed loops using the extrinsic curvature \( K^i_a \) — rather than \( \hat{A}_a^i \) — as a “connection”. This limitation can be overcome in a straightforward fashion using our current strategy. More importantly, this strategy is applicable to all class A Bianchi models, including type IX. Thus, it opens the door to the LQC treatment of all these models in one go.

C. The quantum Hamiltonian constraint

With the connection operator at hand, one can construct the Hamiltonian constraint operator starting either from the general LQG expression (2.19) or the symmetry reduced expression (2.24). We will begin by a small change in the representation of kinematical states which will facilitate this task.

1. A more convenient representation

Ignoring factor ordering ambiguities for the moment, the constraint operator \( \hat{C}_H \) is given by

\[
\hat{C}_H = -\frac{1}{8 \pi G \gamma^2 \Delta^2 p_1} \left[ p_1 p_2 |p_3| \sin \bar{\mu}_1 c_1 \sin \bar{\mu}_2 c_2 + |p_1| p_2 p_3 \sin \bar{\mu}_2 c_2 \sin \bar{\mu}_3 c_3 
+ p_1 |p_2| p_3 \sin \bar{\mu}_3 c_3 \sin \bar{\mu}_1 c_1 \right] - \frac{1}{8 \pi G \gamma^2} \left[ \alpha \bar{\epsilon} p_2 p_3 \sqrt{|p_2 p_3|} \sin \bar{\mu}_1 c_1 
- (1 + \gamma^2) \left( \frac{\alpha p_2 p_3}{2 p_1} \right)^2 \right] + \frac{1}{2} \bar{p}^2 
\]

(3.16)
where for simplicity of notation here and in what follows we have dropped the hats on the \( p_i \) and \( \sin \bar{\mu}_i c_i \) operators. Recall that, classically, the Bianchi II symmetry group reduces to the Bianchi I symmetry group if we set \( \alpha = 0 \). If one sets \( \alpha = 0 \) in (3.16), the last two terms disappear and the operator \( \hat{C}_H \) reduces to that of the Bianchi I model [6] showing explicitly that our construction is a natural generalization of the strategy used there.

To obtain the action of operators corresponding to terms of the form \( \sin \bar{\mu}_i c_i \) we use the same strategy as in [6]. As shown there, it is simplest to introduce dimensionless variables

\[
l_i = \frac{\text{sgn}(p_i) \sqrt{|p_i|}}{(4\pi \gamma \sqrt{\Delta \ell_{pl}^3})^{1/3}}.
\]

Then the kets \(|l_1, l_2, l_3\rangle\) constitute an orthonormal basis in which the operators \( p_k \) are diagonal

\[
p_k |l_1, l_2, l_3\rangle = [\text{sgn}(l_k)(4\pi \gamma \sqrt{\Delta \ell_{pl}^3})^{2/3} l_k^3 |l_1, l_2, l_3\rangle.
\]

Quantum states will now be represented by functions \( \Psi(l_1, l_2, l_3) \). The operator \( e^{i\bar{\mu}_1 c_1} \) acts on them as follows

\[
[e^{i\bar{\mu}_1 c_1} \Psi](l_1, l_2, l_3) = \Psi(l_1 - \frac{1}{|l_2 l_3|}, l_2, l_3) = \Psi(\frac{v - 2 \text{sgn}(l_2 l_3)}{v}, l_1, l_2, l_3),
\]

where we have introduced the variable \( v = 2l_1l_2l_3 \) which is proportional to the volume of the fiducial cell:

\[
\hat{V} \Psi(l_1, l_2, l_3) = [2\pi \gamma \sqrt{\Delta} |v| \ell_{pl}^3 \Psi(l_1, l_2, l_3).
\]

(The \( e^{i\bar{\mu}_1 c_1} \) operator is well-defined in spite of the appearance of \(|l_2 l_3|\) in the denominator; see [6].) The operators \( e^{i\bar{\mu}_2 c_2} \) and \( e^{i\bar{\mu}_3 c_3} \) have analogous action.

We are now ready to write the Hamiltonian constraint explicitly in the \( l_i \)-representation. As noted above, the three terms in the first square bracket on the right hand side of Eq. (3.16) constitute the gravitational part of \( \hat{C}_H \) for the LQC of Bianchi I model\(^4\) and have been discussed in [6]. In the next two sub-sections we will now discuss the last two terms, which are specific to the Bianchi II model.

2. The Fourth term in \( \hat{C}_H \)

Using a symmetric factor ordering, the fourth term becomes

\[
\hat{C}_H^{(4)} = -\frac{\alpha p_2 p_3 \sqrt{|p_2 p_3|}}{16\pi G \gamma^2 \sqrt{\Delta \ell_{pl}^3}} |p_1|^{-1/4} (\xi \sin \bar{\mu}_1 c_1 + \sin \bar{\mu}_1 c_1 \xi) |p_1|^{-1/4}.
\]

(Note that \( p_2 \) and \( p_3 \) commute with the other terms in \( \hat{C}_H^{(4)} \). The operator \( p_1 \) is self-adjoint on \( \mathcal{H}_{\text{kin}}^{\text{grav}} \) whence any measurable function of \( p_1 \) is also a well-defined self-adjoint operator. However, since kets \(|l_1 = 0, l_2, l_3\rangle\) are normalizable in \( \mathcal{H}_{\text{kin}}^{\text{grav}} \), the naive inverse powers of \( \hat{p}_1 \)

\(^4\) There are some minor changes in the action of these three terms since \( \gamma \) is no longer treated as a pseudoscalar (see Appendix A), but these do not affect the discussion.
fail to be densely defined and cannot be self-adjoint. To define inverse powers, as is usual in LQG, we will use a variation on the Thiemann inverse triad identities \[26\]. Classically, we have the identity

\[
|p_1|^{-1/4} = -\frac{i\text{sgn}(p_1)}{2\pi G\gamma} \sqrt{|p_2p_3| \Delta l^2_{\text{Pl}}} e^{-i\bar{\mu}_1c_1} \left\{ e^{i\bar{\mu}_1c_1}, |p_1|^{1/4} \right\}.
\]

(3.22)

which holds for any choice of $\bar{\mu}_1$. Since it is most natural to use the same $\bar{\mu}_1$ that featured in the definition of the connection operator, we will make this choice. Eq (3.22) suggests a natural quantization strategy for $|p_1|^{-1/4}$. Using it and the parity considerations, we are led to the following factor ordering:\[5\]

\[
|p_1|^{-1/4} = -\frac{i\text{sgn}(p_1)}{2\pi G\gamma} \sqrt{|p_2p_3| \Delta l^2_{\text{Pl}}} e^{-i\bar{\mu}_1c_1/2} \frac{1}{i\hbar} \left\{ e^{i\bar{\mu}_1c_1}, |p_1|^{1/4} \right\} e^{-i\bar{\mu}_1c_1/2},
\]

(3.23)

where, as is common in LQC, $\text{sgn}(p_1)$ is defined as

\[
\text{sgn}(p_1) = \begin{cases} +1 & \text{if } p_1 > 0, \\ 0 & \text{if } p_1 = 0, \\ -1 & \text{if } p_1 < 0. \end{cases}
\]

(3.24)

At first it may seem surprising that the expression of $|p_1|^{-1/4}$ involves operators other than $p_1$. It is therefore important to verify that it has the standard desirable properties. First, as one would hope, it is indeed diagonal in the eigenbasis of the operators $\hat{p}_k$:

\[
|p_1|^{-1/4} |l_1, l_2, l_3\rangle = \sqrt{2\text{sgn}(l_1)\sqrt{|l_2l_3|}} \left( \frac{v + \text{sgn}(l_2l_3)}{4\pi \gamma \sqrt{\Delta l^3_{\text{Pl}}}} \right)^{1/6} \left( \sqrt{|v + \text{sgn}(l_2l_3)|} - \sqrt{|v - \text{sgn}(l_2l_3)|} \right) |l_1, l_2, l_3\rangle.
\]

(3.25)

Second, on eigenkets with large volume, the eigenvalue is indeed well-approximated by $p_1^{-1/4}$, whence on semi-classical states it behaves as the inverse of $\hat{p}^{1/4}$, just as one would hope. Thus, (3.25) is a viable candidate for $|p_1|^{-1/4}$. But there are interesting non-trivialities in the Planck regime. In particular, although counter-intuitive, as is common in LQC the operator annihilates states $|l_1, l_2, l_3\rangle$ with $v = 2l_1l_2l_3 = 0$

Finally, note that the operator $\hat{\varepsilon}$ appearing in the expression (3.21) of $\hat{C}_H^{(4)}$ either operates immediately before or after $|p_1|^{-1/4}$. Since $|p_1|^{-1/4}$ annihilates all zero volume states and $\hat{\varepsilon}$ acts on such states as the identity operator, we only need to consider the action of $\hat{\varepsilon}$ on states with nonzero volume. In this case, $\hat{\varepsilon}$ acts as $\text{sgn}(v)$. Therefore the action of $\hat{C}_H^{(4)}$ can be written as:

\[
\left[ \hat{C}_H^{(4)} \Psi \right](l_1, l_2, l_3) = -\frac{i\alpha \pi \sqrt{\Delta l^2_{\text{Pl}}}}{4\pi \gamma \sqrt{\Delta}} \text{sgn}(v) (l_2l_3)^4 \left( \sqrt{|v + \text{sgn}(l_2l_3)|} - \sqrt{|v - \text{sgn}(l_2l_3)|} \right) \left[ \Phi^+(l_1, l_2, l_3) - \Phi^-(l_1, l_2, l_3) \right]
\]

(3.26)

\[5\] In the classical theory, $(L_2L_3)^{1/4} |p_1|^{-1/4}$ is independent of the choice of the elementary cell. As pointed out in [23] the inverse triad operators, by contrast, depend on the choice of the cell. However, one can verify that as we remove the regulator, i.e., take the limit $V \rightarrow \mathbb{R}^3$, as in the classical theory, the limiting $(L_2L_3)^{1/4} |p_1|^{-1/4}$ has a well defined limit.
where
\[ \Phi^\pm(l_1, l_2, l_3) = \left( \sqrt{|v \pm 2\text{sgn}(l_2l_3)|} + \sqrt{|v \pm 2\text{sgn}(l_2l_3)|} \right) \times \left( \text{sgn}(v) + \text{sgn}(v \pm 2\text{sgn}(l_2l_3)) \right) \Psi \left( \frac{v \pm 2\text{sgn}(l_2l_3)}{v} \right) \Phi \bigg|_{l_1, l_2, l_3} \] (3.27)

Recall that in the classical theory the singularity corresponds precisely to the phase space points at which the volume vanishes. Therefore, as in the Bianchi I model, states with support only on points with \( v = 0 \) will be called `singular' and those which vanish at points with \( v = 0 \) will be called regular. The total Hilbert space \( \mathcal{H}_{\text{grav}} \) is naturally decomposed as a direct sum \( \mathcal{H}_{\text{kin}} = \mathcal{H}_{\text{sing}} \oplus \mathcal{H}_{\text{reg}} \) of singular and regular sub-spaces. We will conclude this discussion by examining the action of \( \hat{C}^{(4)}_H \) on these sub-spaces. Note first that in the action (3.21) of \( \hat{C}^{(4)}_H \), the state is first acted upon by the operator \( |p_1|^{-1/4} \). Since this operator annihilates states \( |l_1l_2l_3\rangle \) with \( v = 2l_1l_2l_3 = 0 \), singular states are simply annihilated by \( \hat{C}^{(4)}_H \). In particular this implies that the singular sub-space is mapped to itself under this action. It is clear from (3.27) that if \( \Psi \) is regular, i.e. vanishes on all points with \( v = 0 \), \( \Phi^\pm \) also vanish at these points. Thus the regular sub-space is also preserved by this action. This fact will be used in the discussion of singularity resolution in section III C 3.

Remark: Our definition of the operator \( |p|^{-1/4} \) is not unique; as is common with non-trivial functions of elementary variables, there are factor ordering ambiguities. For example, for \( 0 < n < 1/2 \), we have the classical identity
\[ |p_1|^{n-1/2} = \frac{-i\text{sgn}(p_1)\sqrt{|p_2p_3|}}{8\pi\gamma \sqrt{\Delta l_{\text{Pl}} n}} e^{-i\mu_1 c_1} \left\{ e^{i\mu_1 c_1}, |p_1|^n \right\}. \]

Hence, it is possible to instead define \( \hat{p}_1^{-1/4} \) as
\[ \hat{p}_1^{-1/4} = \left( |p_1|^{n-1/2} \right)^{-1/(4n-2)} \]
where
\[ |p_1|^{n-1/2} = -\frac{4\pi \gamma \sqrt{\Delta l_{\text{Pl}}}^{(2+2n)/3}}{4^n (8\pi \gamma G \sqrt{\Delta l_{\text{Pl}}})^{3/2} n} \text{sgn}(l_1)|l_2l_3|^{1-2n} \left[ |v + \text{sgn}(l_2l_3)|^{2n} - |v - \text{sgn}(l_2l_3)|^{2n} \right]. \]

For \( n \neq 1/4 \), this choice for the operator \( \hat{p}_1^{-1/4} \) is not equivalent to the one we chose. These two choices are both well-defined and admit the same classical limit but they differ in the Planck regime. It is also possible to construct other such inequivalent \( \hat{p}_1^{-1/4} \) candidate operators. For definiteness we have made the `simplest' choice.

3. The fifth term in \( \hat{C}_H \)

Let us now consider the last term in the expression of the gravitational part of the Hamiltonian constraint
\[ \hat{C}^{(5)}_H = \frac{\alpha^2}{32\pi G \gamma^2} (1 + \gamma^2) (p_2p_3)^2 \hat{p}_1^{-2}. \] (3.28)
This term is simpler since it only involves powers of \( p_k \) and we are working in a representation where \( p_k \) are diagonal. From our discussion of the last section, it is natural to set

\[
\hat{p}_1^{-2} := \left( \hat{p}_1^{-1/4} \right)^8,
\]

then we have

\[
\hat{C}_H^{(5)} \Psi(l_1, l_2, l_3) = \frac{8\pi\alpha^2 \Delta(1 + \gamma^2)\hbar \pi^2}{(4\pi\gamma\sqrt{\Delta})^{2/3}} \text{sgn}(l_1)^8 l_2^8 l_3^8 \times \left( \sqrt{|v + \text{sgn}(l_2l_3)|} - \sqrt{|v - \text{sgn}(l_2l_3)|} \right)^8 \Psi(l_1, l_2, l_3).
\]

(3.30)

Again, it is clear that if \( v = 0 \), the wave function is annihilated by this part of the constraint. Also, it follows by inspection that the singular and regular subspaces are both mapped to themselves by the action of \( \hat{C}_H^{(5)} \).

4. Singularity resolution

We can now determine the gravitational part \( \hat{C}_{\text{grav}} \) of the Hamiltonian constraint by combining the results of [6] and Eqs. (3.26) and (3.30). We have:

\[
\hat{C}_{\text{grav}} = \hat{C}_{\text{grav}}^{(BI)} + \hat{C}_{H}^{(4)} + \hat{C}_{H}^{(5)}
\]

(3.31)

where \( \hat{C}_{\text{grav}}^{(BI)} \) is the gravitational part of the Hamiltonian constraint in the Bianchi I model [6]. There is however, a conceptual subtlety. In the classical theory the Hamiltonian density \( C_{\text{grav}}/(L_1L_2L_3)^2 \) is independent of the choice of the elementary cell (where we have to divide by \( (L_1L_2L_3)^2 \) because the lapse corresponding to harmonic time scales as \( (L_1L_2L_3) \) and the Hamiltonian constraint is obtained by integration over the elementary cell \( V \)). As shown in the section V of [6], \( \hat{C}_{\text{grav}}^{(BI)}/(L_1L_2L_3)^2 \) is again independent of the choice of the elementary cell \( V \). However, the two additional terms that are special to the Bianchi II model are not independent of \( V \) because they involve the inverse-triad operators [23]. Nonetheless, in the limit as we take the regulator away, i.e., \( V \to \mathbb{R}^3 \), the operator \( \hat{C}_{\text{grav}}/(L_1L_2L_3)^2 \) has a well-defined limit (see footnote 5). Strictly speaking, in the discussion of Bianchi II quantum dynamics, we have to work with this limit, rather than with operators defined using a fixed cell.

As in the Bianchi I model, the action simplifies if we replace one of the \( l_i \) by \( v \). In the Bianchi I model, it does not matter which of the \( l_i \) is replaced because of the additional symmetry of that model. In the Bianchi II case, while it remains possible to replace any of the \( l_i \), it is simplest to replace \( l_1 \) by \( v \) and represent quantum states as \( \Psi = \Psi(l_2, l_3, v; T) \). This change of variables would be nontrivial if, as in the Wheeler-DeWitt theory, we had used the Lesbegue measure in the gravitational sector. However, it is quite tame here because the norms are defined using a discrete measure. The inner product on \( \mathcal{H}_{\text{kin}}^{\text{grav}} \) is now given by

\[
\langle \Psi_1 | \Psi_2 \rangle_{\text{kin}} = \sum_{l_2, l_3, v} \Psi_1(l_2, l_3, v) \Psi_2(l_2, l_3, v)
\]

(3.32)

and states are symmetric under the action of \( \hat{\Pi}_k \). In Appendix A, we show that, under the action of reflections \( \hat{\Pi}_i \), the operators \( \sin \mu_i c_i \) have the same transformation properties
that $c_i$ have under reflections $\Pi_i$ in the classical theory. As a consequence, $\hat{C}_{\text{grav}}$ is also reflection symmetric. Therefore, its action is well defined on $\mathcal{H}_{\text{grav}}^{\text{kin}}$: $\hat{C}_{\text{grav}}$ is also reflection symmetric. Therefore, its action is well defined on $\mathcal{H}_{\text{grav}}^{\text{kin}}$. In the isotropic case, its analog has been shown to be essentially self-adjoint \cite{30}. In what follows we will assume that \eqref{3.31} is essentially self-adjoint on $\mathcal{H}_{\text{grav}}^{\text{kin}}$ and work with its self-adjoint extension.

It is now straightforward to write down the full Hamiltonian constraint on $\mathcal{H}_{\text{grav}}^{\text{kin}}$:

$$-\hbar^2 \partial_{T}^2 \Psi(l_2, l_3, v; T) = \Theta \Psi(l_2, l_3, v; T) \quad \text{where} \quad \Theta = -2\hat{C}_{\text{grav}}$$ \hspace{1cm} \text{(3.33)}

As in the isotropic case \cite{29}, one can obtain the physical Hilbert space $\mathcal{H}_{\text{phy}}$ by a group averaging procedure and the final result is completely analogous. Elements of $\mathcal{H}_{\text{phy}}$ consist of 'positive frequency' solutions to \eqref{3.33}, i.e., solutions to

$$-i\hbar \partial_T \Psi(l_2, l_3, v; T) = \sqrt{|\Theta|} \Psi(l_2, l_3, v; T),$$ \hspace{1cm} \text{(3.34)}

which are symmetric under the three reflection maps $\Pi_i$, i.e. satisfy

$$\Psi(l_2, l_3, v; T) = \Psi(|l_2|, |l_3|, |v|; T).$$ \hspace{1cm} \text{(3.35)}

The scalar product is given simply by:

$$\langle \Psi_1 | \Psi_2 \rangle_{\text{phys}} = \langle \Psi_1(l_2, l_3, v; T_0) | \Psi_2(l_2, l_3, v; T_0) \rangle_{\text{kin}}$$

$$= \sum_{l_1, l_2, l_3} \bar{\Psi}_1(\vec{l}, T_0) \Psi_2(\vec{l}, T_0)$$ \hspace{1cm} \text{(3.36)}

where $T_0$ is any “instant” of internal time $T$.

We can now address the issue of singularity resolution using general properties of various operators. Recall that the gravitational part of the Hamiltonian constraint operator in the Bianchi I model shares two properties with the fourth and the fifth terms studied above which are specific to the Bianchi II model. First, it annihilates singular states and, second, singular states decouple from the regular states under its action. Therefore the full Bianchi II Hamiltonian constraint also has these two properties. Since the singular states decouple from regular states\footnote{Singular states are in the kernel of $\Theta$ and regular states are orthogonal to the singular ones. From spectral decomposition one expects $\sqrt{\Theta}$ to have the same property. However, to complete this argument, one would have to establish that $\hat{C}_{\text{grav}}$ is essentially self-adjoint and its self adjoint extension also shares this property.}, an initial state in the regular sub-space cannot become singular during evolution. It is in this precise sense that the classical singularity is resolved. Sometimes one considers weaker forms of singularity resolution. For example, it could happen that the evolution of the wave function is always well defined but a regular state can evolve to the singular sub-space. For the Bianchi I and II models, the singularity is resolved in a stronger sense: \textit{Not only is the evolution well defined at all times, but the singular states (are stationary and) decouple entirely from the regular ones.}

5. \textit{The explicit form of the Hamiltonian constraint}

We will conclude by providing an explicit form of the full quantum constraint equation that will be needed in numerical simulations.
Recall that in the Bianchi I model \cite{6} symmetries enabled us to restrict our attention to the positive octant of the 3-dimensional space spanned by \((l_1, l_2, l_3)\). This is again the case for the Bianchi II model. More precisely, elements of \(\mathcal{H}_{\text{kin}}^{\text{grav}}\) are invariant under the three parity maps \(\hat{\Pi}_k\) and, as shown in the Appendix \[ \text{A} \] the Hamiltonian constraint satisfies \(\hat{\Pi}_k \hat{\mathcal{C}}_{\text{grav}} \hat{\Pi}_k = \hat{\mathcal{C}}_{\text{grav}}\). Therefore, knowledge of the restriction of the image \(\hat{\mathcal{C}}_{\text{grav}} \Psi\) of \(\Psi\) to the positive octant suffices to determine \(\hat{\mathcal{C}}_{\text{grav}} \Psi\) completely. In the positive octant, \(\text{sgn}(l_k)\) can only be 0 or 1 which simplifies the action of operators. Therefore, in the remainder of this section we will restrict the argument of \(\hat{\mathcal{C}}_{\mathcal{H}} \Psi\) to the positive octant. The full action is given simply by

\[
(\hat{\mathcal{C}}_{\text{grav}} \Psi)(l_2, l_3, v) = (\hat{\mathcal{C}}_{\text{grav}} \Psi)(|l_2|, |l_3|, |v|).
\]  

(3.37)

Since the singular states are annihilated by \(\hat{\mathcal{C}}_{\text{grav}}\), their evolution is trivial:

\[
\partial^2_T \Psi(l_2, l_3, v = 0; T) = 0.
\]

(3.38)

Non-singular states are physically more relevant. On them, the explicit form of the full constraint is given by:

\[
\partial^2_T \Psi(l_2, l_3, v; T) = \frac{\pi G}{2} \left[ \sqrt{v} \left( (v + 2)\sqrt{v + 4} \Psi^+_{4}(l_2, l_3, v; T) - (v + 2)\sqrt{v} \Psi^+_{0}(l_2, l_3, v; T) \right) 
+ (v - 2)\sqrt{v} \Psi^+_0(l_2, l_3, v; T) + (v - 2)\sqrt{v - 4} \Psi^-_0(l_2, l_3, v; T) \right) 
+ \frac{2i\alpha\sqrt{\Delta}}{(4\pi\gamma\sqrt{\Delta})^{1/3}} (l_2l_3)^{4} \left( \sqrt{v + 1} - \sqrt{|v - 1|} \right) \left( \Phi^- - \Phi^+ \right)(l_2, l_3, v; T) 
+ \frac{16\alpha^2\Delta(1 + \gamma^2)}{(4\pi\gamma\sqrt{\Delta})^{2/3}} (l_2l_3)^{8} \left( \sqrt{v + 1} - \sqrt{|v - 1|} \right)^{8} \Psi(l_2, l_3, v; T) \right]
\]

(3.39)

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

\[
\Psi^\pm_{4}(l_2, l_3, v; T) = \Psi\left( \frac{v + 4}{v} \cdot l_2, \frac{v + 2}{v} \cdot l_3, v \pm 4; T \right) + \Psi\left( \frac{v + 4}{v} \cdot l_2, l_3, v \pm 4; T \right) 
+ \Psi\left( \frac{v + 2}{v} \cdot l_2, \frac{v + 4}{v} \cdot l_3, v \pm 4; T \right) + \Psi\left( \frac{v + 2}{v} \cdot l_2, l_3, v \pm 4; T \right) 
+ \Psi\left( l_2, \frac{v + 2}{v} \cdot l_3, v \pm 4; T \right) + \Psi\left( l_2, \frac{v + 4}{v} \cdot l_3, v \pm 4; T \right),
\]

(3.40)

and

\[
\Psi^\pm_{0}(l_2, l_3, v; T) = \Psi\left( \frac{v + 2}{v} \cdot l_2, \frac{v}{v + 2} \cdot l_3, v; T \right) + \Psi\left( \frac{v}{v + 2} \cdot l_2, \frac{v + 2}{v} \cdot l_3, v; T \right) 
+ \Psi\left( \frac{v}{v + 2} \cdot l_2, \frac{v}{v + 2} \cdot l_3, v; T \right) + \Psi\left( \frac{v}{v + 2} \cdot l_2, l_3, v; T \right) 
+ \Psi\left( l_2, \frac{v}{v + 2} \cdot l_3, v; T \right) + \Psi\left( l_2, \frac{v + 2}{v} \cdot l_3, v; T \right),
\]

(3.41)
while \((\Phi^- - \Phi^+)\) is given by

\[
(\Phi^- - \Phi^+)(l_2, l_3, v; T) = \left(\sqrt{|v - 2 + \text{sgn}(v - 2)|} - \sqrt{|v - 2 - \text{sgn}(v - 2)|}\right) \\
\times \left(1 + \text{sgn}(v - 2)\right)\Psi(l_2, l_3, v - 2; T) \\
- 2(\sqrt{v + 3 - \sqrt{v + 1}})\Psi(l_2, l_3, v + 2; T).
\]

(3.42)

(The imaginary coefficients in (3.39) come from the action of single \(\sin \mu_i c_i\) terms.)

Eq. (3.39) immediately implies that, as in the Bianchi I model, the steps in \(v\) are uniform: the argument of the wave function only involves \(v - 4, v - 2, v, v + 2\) and \(v + 4\). Thus, there is a superselection in \(v\). For each \(\epsilon \in [0, 2)\), let us introduce a lattice \(L_\epsilon\) of points \(v = 2n + \epsilon\) if \(\epsilon\) is 0 or 1 or \(v = n + \epsilon\) otherwise. Then the quantum evolution —and the action of the Dirac observables \(\hat{p}_T\) and \(\hat{V}|_T\) commonly used in LQC— preserves the subspaces \(H^\epsilon_{\text{phy}}\) consisting of states with support in \(v\) on \(L_\epsilon\). The most interesting lattice is the one corresponding to \(\epsilon = 0\) since it includes the classically singular points \(v = 0\).

Finally, it is obvious from (3.39) that in the limit \(\alpha \to 0\) quantum dynamics of the Bianchi II model reduces to that of the Bianchi I model discussed in [6]. In particular, it is possible to obtain the LQC dynamics for the \(k=0\) FRW cosmology from this model by first taking \(\alpha \to 0\) and then following the projection map defined in section IVA in [6].

IV. EFFECTIVE EQUATIONS

In the isotropic models, effective equations have been introduced via two different approaches—the embedding and the truncation methods. Both start by regarding the space of quantum states as an infinite dimensional symplectic manifold—the quantum phase space—which is also equipped with a Kähler structure that descends from the Hermitian inner product on the Hilbert space. In the first method, one finds a judicious embedding of the classical phase space into the quantum phase space which is approximately preserved by the quantum evolution vector field \([27, 28]\). By projecting this vector field into the image of the embedding one obtains quantum corrected effective equations. In the isotropic case these effective equations provide an excellent approximation to the full quantum evolution of states which are Gaussians at late times, even in the \(\Lambda \neq 0\) as well as \(k=\pm 1\) cases where the models are not exactly soluble. In the second method one uses expectation values, uncertainties, and higher moments to define a convenient system of coordinates on the infinite dimensional phase space. The exact quantum evolution equations are then a set of coupled non-linear ordinary differential equations for these coordinates. By a judicious truncation of this system one obtains effective equations containing quantum corrections \([31]\). In its spirit the first method is analogous to the ‘variational principle technique’ used in perturbation theory, in that it requires a judicious combination of art (of selecting the embedding) and science. It is often simpler to use and can be surprisingly accurate. The second method is more systematic, similar in our analogy to the standard, order by order perturbation theory. It is also more general in the sense that it is applicable to a wide variety of states. In this section we will use the first method to gain qualitative insights into leading order quantum effects.

\[7\] The lattice for \(\epsilon \neq 0, 1\) is twice as large as that for \(\epsilon = 0\) or \(\epsilon = 1\) due to the symmetry properties of the wave function.
To obtain the effective equations, without loss of generality we can restrict our attention to the positive octant of the classical phase space (where $\varepsilon = 1$). Then the quantum corrected Hamiltonian constraint is given by the classical analogue of (3.10):

$$\frac{p_T^2}{2} + C_{\text{grav}}^{\text{eff}} = 0,$$

(4.1)

where

$$C_{\text{grav}}^{\text{eff}} = -\frac{p_1 p_2 p_3}{8\pi G \gamma^2 \Delta \ell_p^2} \left[ \sin \bar{\mu}_1 c_1 \sin \bar{\mu}_2 c_2 + \sin \bar{\mu}_2 c_2 \sin \bar{\mu}_3 c_3 + \sin \bar{\mu}_3 c_3 \sin \bar{\mu}_1 c_1 \right] - \frac{1}{8\pi G \gamma^2} \left[ \frac{\alpha (p_2 p_3)^{3/2}}{\sqrt{\Delta \ell_p} p_1^{3/2}} \sin \bar{\mu}_1 c_1 - (1 + \gamma^2) \left( \frac{\alpha p_2 p_3}{2p_1} \right)^2 \right].$$

(4.2)

Using the expressions (3.9) of $\bar{\mu}_k$, it is easy to verify that far away from the classical singularity —more precisely in the regime in which the (gauge fixed) spin connection and the extrinsic curvature are sufficiently small so that $c_k \bar{\mu}_k \ll 1$— the effective Hamiltonian constraint (4.1) is well-approximated by the classical one (2.24).

Since $\sin \theta$ is bounded by 1 for all $\theta$, these equations imply that the matter density $\rho_{\text{matt}} = \frac{p_T^2}{2V^2} = \frac{p_T^2}{2p_1 p_2 p_3}$ satisfies

$$\rho_{\text{matt}} \leq \frac{3}{8\pi G \gamma^2 \Delta \ell_p} + \frac{1}{8\pi G \gamma^2} \left[ \frac{x}{\sqrt{\Delta \ell_p}} - \frac{(1 + \gamma^2)x^2}{4} \right]$$

(4.3)

where we have introduced $x := \alpha \sqrt{p_2 p_3}/p_1^3$. The maximum of the expression in square brackets is attained at $x = 2/(1 + \gamma^2)\sqrt{\Delta \ell_p}$, whence

$$\rho_{\text{matt}} \leq \frac{3 + (1 + \gamma^2)^{-1}}{8\pi G \gamma^2 \Delta \ell_p^2} \approx 0.54 \rho_{\text{Pl}}.$$

(4.4)

Thus, on the constraint surface in the phase space defined by (4.1), the matter energy density is bounded by $0.54 \rho_{\text{Pl}}$. But this bound may be far from being optimal. In all isotropic models, the optimal bound on matter density was found to be $0.41 \rho_{\text{Pl}}$. In the Bianchi I model, available simulations by Vandersloot (private communication) show that the ‘volume bounce’ occurs when matter density is lower than $0.41 \rho_{\text{Pl}}$ because there is also energy density in gravitational waves. It would be interesting to use numerical simulations to find out what happens for generic solutions to the Bianchi II effective equations.

Finally, to obtain the effective equations for each variable, one simply takes its Poisson bracket with the effective Hamiltonian constraint. This gives the effective equations

$$\dot{p}_1 = \gamma^{-1} \left( \frac{p_T^2}{\mu_1} (\sin \bar{\mu}_2 c_2 + \sin \bar{\mu}_3 c_3) + \alpha p_2 p_3 \right) \cos \bar{\mu}_1 c_1,$$

(4.5)

$$\dot{p}_2 = \frac{p_T^2}{\gamma \mu_2} (\sin \bar{\mu}_1 c_1 + \sin \bar{\mu}_3 c_3) \cos \bar{\mu}_2 c_2,$$

(4.6)

$$\dot{p}_3 = \frac{p_T^2}{\gamma \mu_3} (\sin \bar{\mu}_1 c_1 + \sin \bar{\mu}_2 c_2) \cos \bar{\mu}_3 c_3,$$

(4.7)
\[ \dot{c}_1 = -\frac{1}{\gamma} \left[ \frac{p_2 p_3}{\Delta \ell^2_{\text{Pl}}} \left( \sin \bar{\mu}_1 c_1 \sin \bar{\mu}_2 c_2 + \sin \bar{\mu}_1 c_1 \sin \bar{\mu}_3 c_3 + \sin \bar{\mu}_2 c_2 \sin \bar{\mu}_3 c_3 \right) \\
+ \frac{\bar{\mu}_1 c_1}{2} \cos \bar{\mu}_1 c_1 (\sin \bar{\mu}_2 c_2 + \sin \bar{\mu}_3 c_3) - \frac{\bar{\mu}_2 c_2}{2} \cos \bar{\mu}_2 c_2 (\sin \bar{\mu}_1 c_1 + \sin \bar{\mu}_3 c_3) \\
- \frac{\bar{\mu}_3 c_3}{2} \cos \bar{\mu}_3 c_3 (\sin \bar{\mu}_1 c_1 + \sin \bar{\mu}_2 c_2) \right) + (1 + \gamma^2) \alpha^2 \frac{(p_2 p_3)^2}{2 \mu_1^3} \] 
\[ + \frac{\alpha \mu_3}{2 \mu_1} \left( 3 \sin \bar{\mu}_1 c_1 - \bar{\mu}_1 c_1 \cos \bar{\mu}_1 c_1 \right), \quad (4.8) \]

\[ \dot{c}_2 = -\frac{1}{\gamma} \left[ \frac{p_1 p_3}{\Delta \ell^2_{\text{Pl}}} \left( \sin \bar{\mu}_1 c_1 \sin \bar{\mu}_2 c_2 + \sin \bar{\mu}_1 c_1 \sin \bar{\mu}_3 c_3 + \sin \bar{\mu}_2 c_2 \sin \bar{\mu}_3 c_3 \right) \\
- \frac{\bar{\mu}_1 c_1}{2} \cos \bar{\mu}_1 c_1 (\sin \bar{\mu}_2 c_2 + \sin \bar{\mu}_3 c_3) + \frac{\bar{\mu}_2 c_2}{2} \cos \bar{\mu}_2 c_2 (\sin \bar{\mu}_1 c_1 + \sin \bar{\mu}_3 c_3) \\
- \frac{\bar{\mu}_3 c_3}{2} \cos \bar{\mu}_3 c_3 (\sin \bar{\mu}_1 c_1 + \sin \bar{\mu}_2 c_2) \right) - (1 + \gamma^2) \alpha^2 \frac{p_2 p_3^2}{2 \mu_1^3} \] 
\[ + \frac{\alpha p_3}{2 \mu_1} (3 \sin \bar{\mu}_1 c_1 - \bar{\mu}_1 c_1 \cos \bar{\mu}_1 c_1), \quad (4.9) \]

\[ \dot{c}_3 = -\frac{1}{\gamma} \left[ \frac{p_1 p_2}{\Delta \ell^2_{\text{Pl}}} \left( \sin \bar{\mu}_1 c_1 \sin \bar{\mu}_2 c_2 + \sin \bar{\mu}_1 c_1 \sin \bar{\mu}_3 c_3 + \sin \bar{\mu}_2 c_2 \sin \bar{\mu}_3 c_3 \right) \\
- \frac{\bar{\mu}_1 c_1}{2} \cos \bar{\mu}_1 c_1 (\sin \bar{\mu}_2 c_2 + \sin \bar{\mu}_3 c_3) - \frac{\bar{\mu}_2 c_2}{2} \cos \bar{\mu}_2 c_2 (\sin \bar{\mu}_1 c_1 + \sin \bar{\mu}_3 c_3) \\
+ \frac{\bar{\mu}_3 c_3}{2} \cos \bar{\mu}_3 c_3 (\sin \bar{\mu}_1 c_1 + \sin \bar{\mu}_2 c_2) \right) + (1 + \gamma^2) \alpha^2 \frac{p_2^2 p_3}{2 \mu_1^3} \] 
\[ + \frac{\alpha p_2}{2 \mu_1} (3 \sin \bar{\mu}_1 c_1 - \bar{\mu}_1 c_1 \cos \bar{\mu}_1 c_1). \quad (4.10) \]

In the “embedding approach” these effective equations provide the leading-order quantum corrections to the classical equations of motion Eqs. (2.27) – (2.32). It would be very interesting to numerically test if the accuracy they display in the isotropic case for states which are Gaussians at late times carries over to the Bianchi II case.

V. DISCUSSION

In this paper, we analyzed the “improved” LQC dynamics of the Bianchi II model. As in the isotropic and Bianchi I cases, we chose the matter source to be a massless scalar field since it continues to serve as a viable relational time parameter in the classical as well as the quantum theory. It is again rather straightforward to accommodate additional matter fields in this framework.

Our broad strategy is the same as that used in the Bianchi I model [6]. However, because Bianchi II models have anisotropies as well as spatial curvature, holonomies around closed curves are no longer guaranteed to be almost periodic functions of the connection. Hence, one cannot use them to construct the field strength operator on the LQC Hilbert space; a new conceptual and technical input is necessary to define the quantum Hamiltonian constraint operator. We overcame this difficulty by generalizing the strategy used so far [6, 10, 11].
Specifically, we used holonomies around open segments parallel to the fiducial triads $\varepsilon^a$ to define a connection operator. This strategy is also inspired by methods introduced by Thiemann in the full theory [26]. However, because of gauge fixing LQC does not enjoy the manifest diffeomorphism invariance of full LQG. As a consequence, in LQC one needs a principle to fix the ‘length’ of the open segment along which holonomy is evaluated. We required that the ‘length’ be so chosen that the field strength operator constructed from the resulting connection should agree with that constructed from holonomies around closed loops whenever the second construction is available. This guarantees that (apart from ‘tame’ factor ordering ambiguities) the new procedure reduces to the one used in the LQC literature before. Moreover, the strategy of defining the Hamiltonian constraint through this connection operator can be used also in more general contexts. In particular, it enables one to overcome a conceptual limitation of the otherwise complete treatment of the isotropic, $k=−1$ model given in [23, 24]. More importantly, it extends to more general class A Bianchi models. A systematic treatment of the Bianchi IX model along the lines of this paper would be especially interesting.

There is a second —but primarily technical— difference from the Bianchi I case: The Hamiltonian operator now contains inverse powers of $p_1$. This was handled following a general method introduced by Thiemann to define inverse triad operators in LQG [26]. As usual, there is a factor ordering ambiguity. In the main discussion we used the simplest operator which has the same symmetries with respect to parity as its classical counterpart.

After addressing these two issues, we obtained a well defined quantum Hamiltonian constraint and showed that the singularity in Bianchi II models is resolved in the same precise sense as in the FRW and Bianchi I models. The Kinematical Hilbert space $\mathcal{H}_{\text{kin}}^{\text{grav}}$ can be decomposed as $\mathcal{H}_{\text{kin}}^{\text{grav}} = \mathcal{H}_{\text{sing}}^{\text{grav}} \oplus \mathcal{H}_{\text{reg}}^{\text{grav}}$ where states in the singular subspace have support only on configurations with zero volume, while those in the regular sub-space have no support on these singular configurations. The Hamiltonian constraint annihilates states in $\mathcal{H}_{\text{sing}}^{\text{grav}}$ and maps $\mathcal{H}_{\text{reg}}^{\text{grav}}$ to itself. We also provided an explicit form of the Hamiltonian constraint which should be helpful in performing numerical simulations.

Finally, we obtained effective equations using the “embedding method” introduced by Willis [27] and further developed by Taveras [28] in the isotropic case. There, although the assumptions made in the derivation fail in the deep Planck regime, the final equations provide a surprisingly accurate approximation to the full quantum evolution of states which are Gaussians at late times. This holds not only for the exactly soluble $k=0$, $\Lambda = 0$ model but also for the much more complicated $\Lambda \neq 0$ and $k=±1$ models. It would be interesting to see if this phenomenon extends also to Bianchi II models. Furthermore, numerical solutions of these effective equations themselves may be of considerable interest because the simplest upper bound on matter density they lead to is higher than that in all other models studied so far, including Bianchi I. Numerical simulations of effective equations will answer several questions within this approximation. Is the upper bound optimal, i.e., do generic solutions to effective equations come close to saturating it? In the Bianchi I case, numerical simulations by Vandersloot (private communication) revealed that, unlike in the isotropic model, there are several distinct kinds of ‘bounces.’ Roughly, anytime a shear —or a Weyl curvature— scalar enters the Planck regime, quantum geometry repulsion comes into play in a dominant manner and ‘dilutes’ that scalar, preventing a blow up. How do additional terms in the Bianchi II effective equations affect this scenario? Qualitative lessons from numerical simulations would be valuable in developing further intuition for various quantum geometry effects.
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APPENDIX A: PARITY SYMMETRIES

In non-gravitational physics, parity transformations are normally taken to be discrete diffeomorphisms $x_i \rightarrow -x_i$ 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. Therefore these discrete symmetries are no longer meaningful (except in the weak field limit). 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 $v^i$, there is a parity operator $\Pi_v$ which reflects the internal vectors across the 2-plane orthogonal to $v^i$. This operation induces a natural action on triads $e^a_i$, the connections $A^a_i$ and the conjugate momenta $P^a_i =: \left(1/(8\pi G\gamma)\right)E^a_i$ (since they are internal vectors or co-vectors).

The triads $e^a_i$ are proper internal co-vectors. In previous references [6, 32], conventions were such that the spin connection $\Gamma^a_i$ turned out to be an internal pseudo-vector. It was then natural to regard the Barbero-Immirzi parameter $\gamma$ to be a pseudo quantity so that the connection $A^a_i$ has definite parity namely, it transforms as an internal pseudo-vector. This in turn led to the conclusion that $P^a_i$ is also an internal pseudo-vector (as one would expect because it is canonically conjugate to $A^a_i$) [6]. While this is all self-consistent, these conventions lead to two undesirable consequences. First, in the classical theory, it is not possible to reconstruct the triads $e^a_i$ unambiguously starting from the momenta $P^a_i$. Therefore, one cannot recover the space-time geometry unambiguously starting from the Hamiltonian theory. Second, the momenta $P^a_i$ are subject to a non-holonomic constraint which obstructs the passage to quantum theory a la LQG. However, if one sets conventions as in section II A, then $\Gamma^i_a, \gamma, A^i_a$ and $P^a_i$ are all proper quantities and the two difficulties disappear [19]. In the main text we have used this strategy. We now summarize the differences from the Appendix of [6] that it leads to.

In diagonal Bianchi models, we can restrict ourselves just to three parity operations $\Pi_i$. Under their action, the canonical variables $c_i, p_i$ transform as follows:

$$\Pi_1(c_1, c_2, c_3) = (-c_1, c_2, c_3), \quad \Pi_1(p_1, p_2, p_3) = (-p_1, p_2, p_3),$$

(A1)

and the action of $\Pi_2, \Pi_3$ is given by cyclic permutations. Thus, $c^i$ and $p_i$ are proper internal vectors and co-vectors. Under any of these maps $\Pi_i$, the symplectic structure (2.18), the Hamiltonian (2.24), and hence also the Hamiltonian vector field, are left invariant. This is just as one would expect because $\Pi_i$ are simply large gauge transformations of the theory under which the physical metric $q_{ab}$ and the extrinsic curvature $K_{ab}$ do not change. Also, it is clear from the action of (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) $\Pi_i$. Therefore, in the classical theory one can restrict one’s attention just to the positive octant.

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

$$\hat{\Pi}_1 \Psi(l_1, l_2, l_3) = \Psi(-l_1, l_2 l_3),$$

(A2)

etc. What is the induced action on operators? Since

$$\hat{\Pi}_1 \hat{\Pi} \hat{\Pi}_1 (l_1, l_2, l_3) = \hat{\Pi}_1 \left( l_1 \Psi(-l_1, l_2, l_3) \right)$$

$$= -l_1 \Psi(l_1, l_2, l_3),$$

(A3)

we have

$$\hat{\Pi}_1 \hat{\Pi} \hat{\Pi}_1 = -\hat{\Pi}_1.$$  

(A4)

The Hamiltonian constraint operator, modulo factor ordering which is not important here, is given by Eq. (3.16). To calculate its transformation property under parity maps, in addition to (A4), we also need the transformation property of the operators $\sin \bar{\mu}_i c_i$ and $\check{\varepsilon}$ and operators corresponding to inverse powers of $p_1$. Due to the symmetries of type A Bianchi models, to know the properties of $\sin \bar{\mu}_i c_i$ under parity transformations, it is sufficient to calculate $\bar{\Pi}_i \sin \bar{\mu}_i c_i \bar{\Pi}_i$. We have:

$$\bar{\Pi}_1 \sin \bar{\mu}_1 c_1 \bar{\Pi}_1 \Psi(l_1, l_2, l_3) = \frac{1}{2i} \bar{\Pi}_1 \left[ \Psi(-l_1 + \frac{1}{|l_2 l_3|}, l_2, l_3) - \Psi(-l_1 - \frac{1}{|l_2 l_3|}, l_2, l_3) \right]$$

$$= \frac{1}{2i} \left[ \Psi(l_1 + \frac{1}{|l_2 l_3|}, l_2, l_3) - \Psi(l_1 - \frac{1}{|l_2 l_3|}, l_2, l_3) \right]$$

$$= -\sin \bar{\mu}_1 c_1 \Psi(l_1, l_2, l_3),$$

(A5)

whence

$$\bar{\Pi}_1 \sin \bar{\mu}_1 c_1 \bar{\Pi}_1 = -\sin \bar{\mu}_1 c_1.$$  

(A6)

An identical calculation shows that

$$\bar{\Pi}_2 \sin \bar{\mu}_1 c_1 \bar{\Pi}_2 \Psi(l_1, l_2, l_3) = \frac{1}{2i} \bar{\Pi}_2 \left[ \Psi(l_1 - \frac{1}{|l_2 l_3|}, -l_2, l_3) - \Psi(l_1 + \frac{1}{|l_2 l_3|}, -l_2, l_3) \right]$$

$$= \frac{1}{2i} \left[ \Psi(l_1 - \frac{1}{|l_2 l_3|}, l_2, l_3) - \Psi(l_1 + \frac{1}{|l_2 l_3|}, l_2, l_3) \right]$$

$$= \sin \bar{\mu}_1 c_1 \Psi(l_1, l_2, l_3),$$

(A7)

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

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

(A8)

As expected, these transformation properties of $\sin \bar{\mu}_1 c_1$ under $\bar{\Pi}_i$ mirror those of $c_1$ under the three parity operations $\Pi_i$ 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.) Finally, it is clear from Eq. (3.8) that

$$\bar{\Pi}_i \check{\varepsilon} \bar{\Pi}_i = \begin{cases} \check{\varepsilon} \text{ if } v = 0, \\ -\check{\varepsilon} \text{ otherwise,} \end{cases}$$

(A9)
and from Eq. (3.25) that
\[ \hat{\Pi}_i \left| p_1 \right|^{-1/4} \hat{\Pi}_i = \left| p_1 \right|^{-1/4}. \]  
(Note incidentally that this need not be the case for different factor ordering choices in Eq. (3.25).

We can now collect these results to study the transformation property of the Hamiltonian constraint. Consider first the regular subspace \( \mathcal{H}_{\text{reg}}^{\text{grav}} \) of \( \mathcal{H}_{\text{kin}}^{\text{grav}} \) spanned by states which have no support on points with \( v = 0 \). From Eq. (3.16) it follows that the restriction to \( \mathcal{H}_{\text{reg}}^{\text{grav}} \) of the gravitational part of the Hamiltonian constraint is left invariant under \( \hat{\Pi}_i \). Since \( \hat{p}_T^2 \) is manifestly invariant, on the regular sub-space we have
\[ \hat{\Pi}_i \hat{C}_H \hat{\Pi}_i = \hat{C}_H \]  
(A11)

Next, since the gravitational part of the Hamiltonian constraint annihilates the states in the singular sub-space (i.e. those with support only on those points at which \( v = 0 \)), we have
\[ \hat{C}_H \Psi = -\hbar^2 \partial_1^2 \Psi = \hat{\Pi}_i \hat{C}_H \hat{\Pi}_i \Psi. \]  
(A12)

Thus, the Hamiltonian constraint operator is left invariant by all the parity operators, mirroring the behavior of its classical counterpart.

This invariance implies that, given any state \( \Psi \in \mathcal{H}_{\text{kin}}^{\text{grav}} \), the restriction to the positive octant of its image under \( \hat{C}_{\text{grav}} \) determines its image everywhere on \( \mathcal{H}_{\text{kin}}^{\text{grav}} \). This property simplifies calculations and was used to arrive at the form of the Hamiltonian constraint given in (3.39).

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