Loop Quantum Cosmology in Bianchi Type I Models: Analytical Investigation

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Abstract

The comprehensive formulation for loop quantum cosmology in the spatially flat, isotropic model was recently constructed. In this paper, the methods are extended to the anisotropic Bianchi I cosmology. Both the precursor and the improved strategies are applied and the expected results are established: (i) the scalar field again serves as an internal clock and is treated as emergent time; (ii) the total Hamiltonian constraint is derived by imposing the fundamental discreteness and gives the evolution as a difference equation; and (iii) the physical Hilbert space, Dirac observables and semi-classical states are constructed rigorously. It is also shown that the state in the kinematical Hilbert space associated with the classical singularity is decoupled in the difference evolution equation, indicating that the big bounce may take place when any of the area scales undergoes the vanishing behavior. The investigation affirms the robustness of the framework used in the isotropic model by enlarging its domain of validity and provides foundations to conduct the detailed numerical analysis.

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References
I. INTRODUCTION

The loop quantum cosmology (LQC) in the spatially flat, isotropic model was recently investigated in detail \([1]\). (For a brief review, see \([2]\).) That investigation introduced a conceptual framework to construct the physical sector and gave the technical tools to systematically explore the effects of quantum geometry both on the gravitational and matter sectors. With a massless scalar field as the matter source, the analysis led to the significant results: (i) the scalar field was shown to serve as an internal clock, thereby providing an explicit realization of the "emergent time" idea; (ii) the physical Hilbert space, Dirac observables and semi-classical states were constructed rigorously; and (iii) the Hamiltonian constraint was solved numerically, showing that in the backward evolution of states which are semi-classical at late times, the big bang is replaced by a quantum bounce. Furthermore, thanks to the non-perturbative, background independent methods, the quantum evolution is deterministic across the deep Planck regime.

These results are attractive and affirm the assertion that the quantum geometry effects of loop quantum gravity (LQG) hold a key to many long standing questions \([3, 4, 5, 6, 7]\). The detailed investigation enriches our understanding of quantum geometry effects both in semi-classical and Planck regimes. However, it has a serious drawback: the critical value \(\rho_{\text{crit}}\) of the matter density at which the bounce occurs can be made arbitrarily small by increasing the momentum \(p_\phi\) of the scalar filed (which is a constant of motion). This is seriously problematic since large values of \(p_\phi\) are permissible and even preferred for semi-classical states at late times and it is physically unreasonable to expect that quantum corrections significantly modify the classical predictions at low matter densities.

A careful consideration urges that this unpleasant feature is just the artifact of approximation schemes and should be overcome by modifying the definition of the constraint operator in a more sophisticated way. In \([8]\), the new Hamiltonian constraint was constructed, based on the same principles used in \([1, 2]\) but improved by a more direct implementation of the underlying physical ideas. The new method retains all the attractive features while resolves the major weakness: in the improved dynamics, the big bounce occurs precisely when the matter density enters the Planck regime, regardless of the value of \(p_\phi\) and other initial conditions.

The investigations \([1]\) and \([8]\) altogether provide a solid foundation for analyzing physical issues of LQC. However, one of the limitations in this formulation is that it is obtained in a specific mini-superspace model and thus the domain of validity is restricted. In order to test the robustness of this framework, it is necessary to apply the methodology to more general situations. The next step is to consider Bianchi I model, the simplest case of homogeneous, anisotropic models. In classical general relativity, the generic approach to the initial singularity is usually understood in terms of the Belinsky-Khalatnikov-Lifshitz (BKL) scenario. In this scenario, along with the Bianchi IX model, the Kasner solution of vacuum Bianchi I model plays a pivotal role for the infinite fragmentation of the homogeneous patches close to the singularity \([9, 10]\). Therefore, a detailed construction of Bianchi I model (with or without matter source) in quantum theory could provide a tool to explore the quantum effect near the classical singularity in generic cases. Moreover, a better understanding of anisotropic Bianchi I models may also shed light on how the isotropy appears in anisotropy. For example, we can ask what kinds of semi-classical (coherent) states in Bianchi I model give rise to the isotropic symmetry, either exactly or approximately. Since so far there is no systematic procedure which leads us to the dynamics of the symmetry reduced theory from
that of the full theory of LQG, understanding the isotropy in the anisotropic framework could give a useful insight into symmetry reduction.

In anisotropic models, the main structural difference from the isotropic case is that the operator \( \Theta \) used in [1, 2, 8] is no longer positive definite. However, a detailed analysis shows that what matters is just the operator \( \Theta_+ \), obtained by projecting the action of \( \Theta \) to the positive eigenspace in its spectral decomposition. Therefore, most analytical structures should go through without a major modification.

The purpose of this paper is to give a detailed analytical investigation of LQC with a massless scalar field in Bianchi I model. Both the precursor strategy ("\( \phi \)-scheme") used in [1] and the improved strategy ("\( \bar{\phi} \)-scheme") used in [8] are applied and reconstructed for the Bianchi I model. The analytical issues are investigated in detail and the parallel results are reproduced. In particular, the scalar field again serves as an internal clock, the physical Hilbert space with the inner product is constructed such that Dirac observables are all self-adjoint and thereby the forms of expectation values and uncertainties of Dirac observables are formulated. Meanwhile, the corresponding Wheeler-DeWitt (WDW) theory is studied and by analogy the semi-classical states for LQC are constructed in both schemes, which match the semi-classical states for WDW at late times.

However, since Bianchi I models have more variety, there are new features significantly different from those in isotropic models and more careful consideration is needed. In the classical dynamics, apart from the solutions which have the similar characteristics to those in isotropic models (i.e., expanding or contracting in all three directions), the Bianchi I model with a massless scalar also admits "Kasner-like" solutions (namely, expanding in two directions while contracting in the other direction or the opposite way around). The Kasner-like solution with two expanding and one contracting directions eventually encounters the "Kasner-like singularity" (a given regular cubical cell stretches as an infinitely long line) in the backward evolution. When the quantum correction is taken into account, according to the implications from the decoupling of the problematic state in the difference evolution equation, we anticipate that the singularity (Kasner-like or not) is resolved and might be replaced by the big bounce. In the Kasner-like case, the big bounce could occur as many as three times, not just once, whenever the corresponding classical solution undergoes vanishing behavior of the area scale factors. Furthermore, in \( \bar{\phi} \)-scheme, the bounce is expected to happen at the moment when the directional factor \( \varrho_I := \frac{\nu_2^2}{|p_I|^3} \) (which plays the same role as the matter density does in the isotropic case) in any of the three diagonal directions \( (p_I \) is the area scale factor in the direction \( I \)) approaches the Planck regime of \( \mathcal{O}(\hbar \ell_{Pl}^4) \) (\( \ell_{Pl} \) is the Planck length), irrespective of the value of \( p_\phi \). In order to conclusively show that this anticipation is indeed the case, we need to conduct a thorough numerical investigation to reveal more phenomenological ramifications due to quantum geometry effects in the Bianchi I model. With the analytical foundation at hand, we are ready to investigate the effective dynamics and numerics, which we wish to study in more detail in a separate paper [11]. (Some results for the effective dynamics have been studied in [12].)

This paper is organized as follows. In Section II we summarize the results of the classical dynamics of the anisotropic Bianchi I cosmology with a massless scalar source. In Section III the Bianchi models are expressed in terms of Ashtekar variables and the phase space of the diagonal Bianchi models is constructed. In particular, the Hamiltonian constraint in Bianchi I model is given in terms of the diagonal variables \( c^I \) and \( p_I \) and serves as the staring point of the whole formulation. Section IV deals with the kinematical structure, highlighting the construction using holonomies to replace connection variables. The gravitational part of
The Hamiltonian constraint is derived in Section V with the quantum discreteness imposed by ℏµ-scheme. The WDW theory is studied in Section VI to show that the singularity is not resolved with WDW equation and to offer a systematic method to construct the physical sector, which then can be heuristically modified for the context of LQC. In Section VII the analytical issues in LQC are studied in detail: the total Hamiltonian constraint is derived and gives the evolution as a difference equation; the state in the kinematical Hilbert space associated with the classical singularity is completely decoupled in the difference evolution equation; and finally the Dirac observables are recognized and the physical Hilbert space is constructed with the physical inner product. Section IV – Section VII complete the analytical investigation for the precursor strategy (ℏµ-scheme). The organization of this part deliberately parallels that of [1] and the notations are also used in the similar manner. The procedures in Section V – Section VII are then repeated all over again with appropriate modifications for the improved strategy (¯µ-scheme) in Section VIII. Finally, the results of this paper and outlooks for further research are discussed in Section IX.

Some technical details and related topics are supplemented in the appendices. The detailed calculation for the WDW semi-classical states is shown in Appendix A. The issues to obtain the formulation for the isotropic model by direct inspection from the anisotropic results are discussed in Appendix B. The comparison with the results of [1, 2, 8] and their subtle differences are also remarked.

II. CLASSICAL DYNAMICS OF THE BIANCHI I MODEL

The Bianchi I model without matter source (Kasner model) has been quantized in the context of LQC in [5], as has the isotropic model with massless scalar source in [1, 2, 8]. In order to study the LQC in Bianchi I model in the presence of massless scalar field, we first have to figure out its classical dynamics and solutions. This has been done in [13], and the results are briefly outlined as follows.

The Hilbert action for the cosmology with a massless scalar filed ϕ minimally coupled to the gravity is given by

\[ S = S_{\text{grav}} + S_\phi = \frac{1}{8\pi G} \int d^4x \sqrt{-g} R - \frac{1}{2} \int d^4x \sqrt{-g} g^{\mu\nu} \phi_{,\mu} \phi_{,\nu}. \]  

(2.1)

In the Bianchi I model, we can take the spacetime metric to be the form

\[
g_{\mu\nu} = \begin{pmatrix}
-n^2(t) & 0 & 0 & 0 \\
0 & a_1^2(t) & 0 & 0 \\
0 & 0 & a_2^2(t) & 0 \\
0 & 0 & 0 & a_3^2(t)
\end{pmatrix}
\]  

(2.2)

and the homogeneous field \( \phi(\vec{x}, t) = \phi(t) \) to be independent of the spatial coordinates. We then have the Hamiltonian constraint

\[
H = C_{\text{grav}} + C_\phi = \pi G \left( -\frac{2\pi_1 \pi_2}{a_3} - \frac{2\pi_1 \pi_3}{a_2} - \frac{2\pi_2 \pi_3}{a_1} + \frac{a_1 \pi_1^2}{a_2 a_3} + \frac{a_2 \pi_2^2}{a_1 a_3} + \frac{a_3 \pi_3^2}{a_1 a_2} \right) + \frac{p_\phi^2}{2a_1 a_2 a_3} = 0, \]  

(2.3)
where \( \pi_i \) are the conjugate momenta of \( a_i \) and \( p_\phi \) is the conjugate momentum of \( \phi \), which satisfy the canonical relations

\[
\{a_i, \pi_j\} = \delta_{ij} \quad \text{and} \quad \{\phi, p_\phi\} = 1.
\]  

(2.4)

The general solution is given by

\[
a_i(t) = a_{i,o} \left( \frac{\tau}{\tau_o} \right)^{\kappa_i} = a_{i,o} \left( \frac{n_o t + \int_0^t dt_2 \int_0^{t_2} dt_1 \lambda(t_1) + \tau_o}{\tau_o} \right)^{\kappa_i},
\]  

(2.5)

and

\[
\phi(t) = \phi_o + \frac{\kappa_\phi}{\sqrt{4\pi G}} \ln \left( \frac{n_o t + \int_0^t dt_2 \int_0^{t_2} dt_1 \lambda(t_1) + \tau_o}{\tau_o} \right),
\]  

(2.6)

where \( \tau \) is the proper time defined through \( d\tau = n(t)dt \), \( \lambda := \dot{n} \equiv \frac{dn}{dt} \) is a positive but otherwise arbitrary function of \( t \) and the constants \( \kappa_i, \kappa_\phi \) satisfy the constraint:

\[
\kappa_1 + \kappa_2 + \kappa_3 = 1 \quad \text{and} \quad \kappa_1^2 + \kappa_2^2 + \kappa_3^2 + \kappa_\phi^2 = 1.
\]  

(2.7)

Since the Hamiltonian is independent of \( \phi \), the momentum \( p_\phi \) is a constant of motion, which is given by

\[
p_\phi = \frac{a_{1,o} a_{2,o} a_{3,o}}{\tau_o} \sqrt{\frac{1}{8\pi G}} \kappa_\phi := \hbar \sqrt{8\pi G K \kappa_\phi}.
\]  

(2.8)

The complete set of solutions will be over-counted unless we fix the constant ratio \( a_{1,o} a_{2,o} a_{3,o}/\tau_o \); thereby we introduce the dimensionless constant \( K \), which is to be fixed. Note that \( \phi \) is a monotonic function of \( t \) and thus it can be used as the internal time. Expressed in terms of the internal time \( \phi \), the solution reads as

\[
a_i(\phi) = a_{i,o} e^{\sqrt{8\pi G \kappa_\phi}(\phi - \phi_o)},
\]  

(2.9)

where the dependence on the coordinate time \( t \) is completely eliminated and only the correlation between the dynamical variables \( a_i \) and \( \phi \) is truly physical! This realizes the idea of emergent time [14] and shows that one can employ some subset or combination of dynamical fields as an internal clock [15]. Later in Section VI A, Section VII B and Section VIII D it will be shown that \( \phi \) is well-suited to be emergent time also in the quantum theory (for both WDW theory and LQC).

**Remark:** If without any matter sources, the classical dynamics of vacuum Bianchi I model yields the standard Kasner solution:

\[
ds^2 = -dt^2 + t^{2\kappa_1} dx_1^2 + t^{2\kappa_2} dx_2^2 + t^{2\kappa_3} dx_3^2,
\]  

(2.10)

where \( \kappa_1, \kappa_2, \kappa_3 \) are constants subject to the constraint:

\[
\kappa_1 + \kappa_2 + \kappa_3 = 1 \quad \text{and} \quad \kappa_1^2 + \kappa_2^2 + \kappa_3^2 = 1.
\]  

(2.11)

\[1\] The choice of \( K \) is in fact a gauge fixing. Change of \( K \) is equivalent to the rescaling: \( \kappa_i \to K \kappa_i \) and \( \kappa_\phi \to K \kappa_\phi \) with the new constraint: \( \kappa_1 + \kappa_2 + \kappa_3 = K \) and \( \kappa_1^2 + \kappa_2^2 + \kappa_3^2 + \kappa_\phi^2 = K^2 \). The rescaled \( \kappa_i \) and \( \kappa_\phi \) still yield the same evolution equation with respect to the internal time \( \phi \) as the rescaling does not change (2.9).
With the exception of the trivial Minkowskian solutions (where two of \(\kappa_i\) vanish), all solutions have two of \(\kappa_i\) positive and the other negative, which therefore lead to the “Kasner singularity”\(^2\) at \(t = 0\) and the “planar collapse”\(^3\) at \(t = \infty\). Now with the massless scalar source introduced, the solution \((2.9)\) with the constraint \((2.7)\) are the modifications of \((2.10)\) and \((2.11)\) and it also admits “Kasner-like” solutions (which thereby give the “Kasner-like” singularity and planar collapse) except that the role of \(t\) is replaced by the internal time \(\phi\). On the other hand, because of \(\kappa_\phi\), we also have nontrivial solutions with \(\kappa_i\) all positive, which are not allowed for standard Kasner solutions. These “Kasner-unlike” solutions have only a (Kasner-unlike) singularity\(^4\) but no planar collapse and behave quite the same as the isotropic solution. In particular, the constraint with \(\kappa_1 = \kappa_2 = \kappa_3 = 1/3\) reproduces the isotropic solution. □

III. BIANCHI MODELS IN ASHTEKAR VARIABLES

In the construction of LQC, so far, quantum gravity has mostly been analyzed in mini- or midi-superspace models which are obtained by ignoring an infinite number of degrees of freedom of the full theory. That is, the canonical dynamical variables are enormously reduced by the symmetry and only a finite number of relevant degrees of freedom are preserved and quantized. This strategy has been used in \([4]\) and formulated rigorously in \([6]\) for the isotropic models; it was also extended to diagonal Bianchi class A models (the subclass of Bianchi types I, II, VIII and IX, or referred as “type D”) in \([5]\). In this section, we follow and outline the ideas of \([16]\) to describe the Bianchi models in Ashtekar variables and end up with the Hamiltonian constraint for the Bianchi I model in terms of the diagonal variables \(c^l\) and \(p_I\).

A. The Description with Ashtekar Variables

Bianchi cosmologies are homogeneous cosmological models, in which there is a foliation of spacetime: \(M = \Sigma \times \mathbb{R}\) such that \(\Sigma\) is space-like and there is a transitive isometry group freely acting on \(\Sigma\). This means that we have the Killing fields on \(\Sigma\). We can choose a fiducial triad of vectors \(\mathring{e}_i^a\) and a fiducial co-triad of covectors \(\mathring{\omega}^i_a\) that are left invariant by the action of the Killing fields. The fiducial 3-metric is given by the co-triad \(\mathring{\omega}^i_a\):

\[
\mathring{q}_{ab} = \mathring{\omega}^i_a \mathring{\omega}^j_b \delta_{ij}. \tag{3.1}
\]

These bases \(\mathring{e}_i^a\) and \(\mathring{\omega}^i_a\) satisfy the relations:

\[
[q_i, q_j]^a = C_{ij}^k q^a_k, \tag{3.2}
\]

\[
2D_{[a} \mathring{\omega}_{b]}^i = -C_{jk}^i \mathring{\omega}^j_{a} \mathring{\omega}^k_{b}, \tag{3.3}
\]

\(^2\) At the “Kasner(-like) singularity”, a given regular cubical cell is stretched as a linear line, infinitely long in one direction and infinitely thin in the other two.

\(^3\) “Planar collapse” means that a given regular cubical cell is stretched as a planar piece, infinitely large in two directions and infinitely thin in the other one. This is however not a spacetime singularity, since the spacetime curvature goes to zero (instead of infinity) when Kasner-like solutions evolve to the far future.

\(^4\) At the “Kasner-unlike singularity”, a given regular cubical cell contracts to a point.
where $C_{ij}^k$ are the structure constants of the above mentioned isometry group. The classification of these structure constants leads to a classification of the homogeneous spaces. The case that we study in this paper is Bianchi I type, in which the structure constants $C_{ij}^k$ all vanish.

The Ashtekar variables consist of the canonical pairs $\tilde{E}^a_i$ and $A_a^i$. The variables $\tilde{E}^a_i$ are densitized triads and the connections $A_a^i$ are defined by

$$A_a^i = \Gamma_a^i - \gamma K_a^i,$$

where $\Gamma_a^i = \epsilon^i_j k \Gamma_{ak}^j$ with $\Gamma_{ak}^j = \frac{1}{2} \epsilon_b^j (\partial_a e_b^j - \partial_b e_a^j + e_c^j e_{al} \partial_b e_c^l)$ the spin connection of the physical triad $e_i^a$; $K_a^i = K_{ab} E^b_i = q^{-1/2} K_{ab} E^b_i$ with $K_{ab}$ the extrinsic curvature of the 3-surface and $q$ the determinant of the 3-metric; and $\gamma$ is the Barbero-Immirzi parameter. In the context of Bianchi models, it is more convenient to consider the variables:

$$E^i_j := o_{q^{-1/2}} \omega_a^i \tilde{E}^a_j,$$

$$A^i_j := A_a^j \omega_a^i.$$

They are essentially the same as the above canonical variables, but stripped of all the complicated but fixed spatial dependence enforced by the Bianchi symmetry. Conversely, we have

$$\tilde{E}^a_i = \sqrt{q} E^i_j \omega_j^a,$$

$$A_a^i = A^i_j \omega_j^a.$$

These matrices $E^i_j$ and $A^i_j$ depend only on time (due to spatial homogeneity) and are our reduced canonical variables. Thus as expected, the number of degrees of freedom (in the configuration space) has been reduced from 9 per space point to just 9 globally. The Gauss, vector and Hamiltonian constraints in terms of these reduced variables are expressed respectively as

$$G^i = C_{jk}^j E^{ki} + G \epsilon^{ijk} A_{mj} E^m_k = 0,$$

$$V_k = -E^j_i A^m_i C_{jk}^m + G \epsilon^{imn} E^i_j A_{jm} A_{kn} = 0,$$

$$S = \epsilon^{ijk} C_{mn}^p E^m_i E^n_j A_{pk} + GE^m_i E^n_j (A^i_m A^j_n - A^j_n A^m_i) = 0,$$

where $\gamma = i$ is used in the last line for the Hamiltonian constraint.

**B. Phase Space in the Diagonal Bianchi Models**

For the diagonal Bianchi class A models, one can fix the gauge of the $SO(3)$ rotation so that $A^i_j$ and $E^i_j$ are diagonalized:

$$\tilde{c}^i = \Lambda^i_{(I)} A^i_j \Lambda_j^{(I)}, \quad \tilde{p}^I = \Lambda^i_{(I)} E^i_j \Lambda_j^{(I)},$$

where $\Lambda^i_{(I)}$ is the $SO(3)$ rotation matrix and $\Lambda_i^{(I)}$ is its inverse.\(^{5}\) In this gauge, (3.7) and (3.8) are identically satisfied and the phase space is reduced to 6-dimensional and labeled by

\(^{5}\) In this paper, the Einstein convention is adopted: the indices repeated on both upper and lower scripts are summed. When Einstein convention is not wanted, those indices which are repeated on both scripts but not to be summed are parenthesized.
\( \tilde{c}^I \) (the diagonalized entries of \( A_j^j \)) and \( \tilde{p}_I \) (the diagonalized entries of \( E_i^j \)) with the single constraint \( S = 0 \). In the diagonal components the symplectic structure is given by

\[
\{ \tilde{c}^I, \tilde{p}_J \} = 8\pi\gamma GV_o \delta^I_J, \tag{3.11}
\]

where \( V_o = ^oL_1^oL_2^oL_3 \) is the volume of the “unit cell” \( V \) adapted to the fiducial triad and \( ^oL_I \) are the lengths of the edges of this cell with respect to \( ^oq_{ab} \). (For simplicity, we assume that this cell is rectangular with respect to \( ^oq_{ab} \).)

In the passage from the full to the reduced theory, we introduced a fiducial metric \( ^oq_{ab} \). There is a freedom in rescaling the diagonal entries of this metric by constants: \( ^oq_{ii} \mapsto k_i^2 ^oq_{ii} \) for \( i = 1, 2, 3 \). Under this rescaling, the variables \( \tilde{c}^I, \tilde{p}_I \) transform correspondingly via \( \tilde{c}^I \mapsto k_i^{-1} \tilde{c}^{(I)} \) and \( \tilde{p}_I \mapsto k_2^{-1} k_3^{-1} \tilde{p}_I \) and so on. Since rescaling of the fiducial metric does not change physics, \( \tilde{c}^I \) and \( \tilde{p}_I \) do not have direct physical meaning and it is convenient to introduce the new variables

\[
c^I = ^oL_{(I)} \tilde{c}^{(I)} \quad \text{and} \quad p_1 = ^oL_2^oL_3\tilde{p}_1, \quad p_2 = ^oL_1^oL_3\tilde{p}_2, \quad p_3 = ^oL_1^oL_2\tilde{p}_3, \tag{3.12}
\]

which is independent of the choice of the fiducial metric \( ^oq_{ab} \). This is equivalent to the relation

\[
\sqrt{^oq} \tilde{c}^{(I)} \tilde{p}_{(I)} = \sqrt{^oq} c^{(I)} p_{(I)}. \tag{3.13}
\]

In terms of the new variables, the canonical relation is

\[
\{ c^I, p_J \} = 8\pi\gamma G \delta^I_J. \tag{3.14}
\]

The relation between the densitized triad and the 3-metric is given by \( qq^{ab} = \delta^{ij} \tilde{E}^a_i \tilde{E}^b_j \), which leads to

\[
p_1 = (a_2 a_3) \text{sgn}(a_1 a_2 a_3), \quad p_2 = (a_1 a_3) \text{sgn}(a_1 a_2 a_3), \quad p_3 = (a_1 a_2) \text{sgn}(a_1 a_2 a_3), \tag{3.15}
\]

where \( a_i \) are the scale factors in the metric of (2.2). Comparing the canonical relations (2.4) and (3.14) with the help of (3.15), we have

\[
c^1 = 4\pi\gamma G \left( \frac{a_1}{a_2 a_3} \pi_1 - \frac{1}{a_3} \pi_2 - \frac{1}{a_2} \pi_3 \right) \text{sgn}(a_1 a_2 a_3),
\]

\[
c^2 = 4\pi\gamma G \left( -\frac{1}{a_3} \pi_1 + \frac{a_2}{a_1 a_3} \pi_2 - \frac{1}{a_1} \pi_3 \right) \text{sgn}(a_1 a_2 a_3),
\]

\[
c^3 = 4\pi\gamma G \left( -\frac{1}{a_2} \pi_1 - \frac{1}{a_1} \pi_2 + \frac{a_3}{a_1 a_2} \pi_3 \right) \text{sgn}(a_1 a_2 a_3). \tag{3.16}
\]

C. The Hamiltonian Constraint in Bianchi I Models

The gravitational part of the Hamiltonian constraint is given by

\[
C_{grav} = q^{-1/2} G_{ab} \tilde{n}^a_i \tilde{n}^b_i = \frac{1}{2\sqrt{q}} \left( ^{(3)} R - K_{ab} K^{ab} + (K_a^a)^2 \right). \tag{3.17}
\]

For Bianchi I models, the spatial slice is flat and thus the intrinsic curvature \( ^{(3)} R = 0 \) and the spin connection of the triad \( \Gamma_a^i = 0 \), which follows \( A_a^i = -\gamma K_a^i \). Consequently, we have

\[
K_a^b = K_a^i \tilde{E}_i^b = -\frac{1}{\sqrt{q}} A_a^i \tilde{E}_i^b = -\frac{1}{\gamma \sqrt{q}} A_a^i \gamma \tilde{E}_i^b = -\frac{1}{\gamma \sqrt{q}} A_a^i \gamma \tilde{E}_i^b \tag{3.18}
\]
and
\[ C_{\text{grav}} = \frac{1}{\gamma^2 q^{3/2}} \left( E^i E^j A_m A_n - E^m E_{nj} A_i A^j \right). \] (3.19)

In the gauge that \( A^i_j \) and \( E^i_j \) are diagonal, the Hamiltonian reads as
\[ C_{\text{grav}} = \frac{2}{\gamma^2 q^{3/2}} \left( c^1 \tilde{p}_1 c^2 \tilde{p}_2 + c^1 \tilde{p}_1 c^3 \tilde{p}_3 + c^2 \tilde{p}_2 c^3 \tilde{p}_3 \right) \]
\[ = \frac{2}{\gamma^2 \sqrt{q}} \left( c^1 p_1 c^2 p_2 + c^1 p_1 c^3 p_3 + c^2 p_2 c^3 p_3 \right). \] (3.20)

[Note that \( C_{\text{grav}} \) in (3.20) is proportional to \( S \) in (3.9) up to the factor \( q^{-3/2} \) with \( C_{ij} = 0 \).

By the identities (3.15), (3.16) and \( \sqrt{q} = |a_1 a_2 a_3| \), (3.20) becomes
\[ C_{\text{grav}} = 16 \pi^2 G^2 \left( \frac{2 \pi^2 p_1}{a_3} + \frac{2 \pi^2 p_3}{a_2} + \frac{2 \pi^2 p_3}{a_1} - \frac{a_1 \pi^2}{a_2 a_3} - \frac{a_2 \pi^2}{a_1 a_3} - \frac{a_3 \pi^2}{a_1 a_2} \right) \operatorname{sgn}(a_1 a_2 a_3), \] (3.21)
which is exactly the same as the gravitational part in (2.3) up to an overall constant factor.

Fixing the difference of the overall factors for \( C_{\text{grav}} \) used in (2.3) and in (3.21) and referring to (3.20), we end up with the Hamiltonian constraint in terms of the diagonal variables \( c^i \) and \( p_i \):
\[ H = C_{\text{grav}} + C_\phi \]
\[ = -2 \frac{\gamma^2}{\gamma^2} \left( c^1 p_1 c^2 p_2 + c^1 p_1 c^3 p_3 + c^2 p_2 c^3 p_3 \right) \frac{1}{\sqrt{|p_1 p_2 p_3|}} + 8 \pi G \frac{1}{\sqrt{|p_1 p_2 p_3|}} p_\phi^2. \] (3.22)

In the new variables, the classical solution (2.3) now reads as
\[ p_1(\phi) = p_{1,o} e^{\sqrt{8 \pi G} \left( \frac{\alpha + \beta}{\kappa} \right) (\phi - \phi_0)} = p_{1,o} e^{\sqrt{8 \pi G} \left( \frac{1 - \frac{3}{2}}{\kappa} \right) (\phi - \phi_0)}, \]
\[ p_2(\phi) = p_{1,o} e^{\sqrt{8 \pi G} \left( \frac{\alpha + \beta}{\kappa} \right) (\phi - \phi_0)} = p_{2,o} e^{\sqrt{8 \pi G} \left( \frac{1 - \frac{3}{2}}{\kappa} \right) (\phi - \phi_0)}, \]
\[ p_3(\phi) = p_{1,o} e^{\sqrt{8 \pi G} \left( \frac{\alpha + \beta}{\kappa} \right) (\phi - \phi_0)} = p_{3,o} e^{\sqrt{8 \pi G} \left( \frac{1 - \frac{3}{2}}{\kappa} \right) (\phi - \phi_0)}. \] (3.23)

**Remark:** The Hamiltonian constraint (3.22) reduces to that of the isotropic model (as given in 4) if we further impose the isotropy condition \( c^1 = c^2 = c^3 = c \) and \( p_1 = p_2 = p_3 = p \) with the canonical structure \( \{c, p\} = 8 \pi G / 3 \).

**IV. KINEMATICS: QUANTIZATION**

In this section, we follow the lines in [6] and generalize the procedures to seek the quantum kinematics for Bianchi I models. Elementary variables and the representation of their algebra are obtained in Section IV A and Section IV B. In Section IV C, the triad operators are constructed in terms of holonomies; the fact that the eigenvalues of the triad operators are bounded above is discussed, suggesting that the classical singularity could be resolved by the quantum geometry.
A. Elementary Variables

Before quantization, we should single out the “elementary functions” on the classical phase space which are to be lifted to their quantum counterparts. In the full theory, the configuration variables are constructed from holonomies $h_\varepsilon(A)$ associated with edges $\varepsilon$ and momentum variables $E(S,f)$, which are momenta $E$ smeared with test fields $f$ on 2-surfaces. In Bianchi I models, however, because of homogeneity, we do not need all edges $\varepsilon$ and surfaces $S$. Symmetric connection $A$ in $\mathcal{A}_S$ can be recovered by knowing holonomies $h_I$ along the edges $e_I$, which lie along straight lines in the “diagonal” directions (for $I = 1,2,3$) in $\Sigma$. Similarly, it is sufficient to smear triads only on the rectangular surfaces of the elementary cell $\mathcal{V}$ (with respect to $q_{\alpha\beta}$).

The $SU(2)$ holonomy along $e_I$ in the diagonal direction $I$ is given by:

$$h_I(A,\mu_I) := \mathcal{P} \exp \int_{e_I} A = \exp(-\frac{i}{2}\mu_I c(I)\sigma(I))$$

$$= \cos \left( \frac{\mu_I c(I)}{2} \right) + 2 \sin \left( \frac{\mu_I c(I)}{2} \right) \tau(I) , \quad (4.1)$$

where $2i\tau_I = \sigma_I$ with $\sigma_I$ the Pauli matrices and $\mu_I \in (-\infty, \infty)$ (and $\mu_I^J L_I$ is the oriented length of the edge with respect to $q_{\alpha\beta}$). According to Peter-Weyl theorem, a basis on the Hilbert space of $L_2$ functions on $SU(2)$ is given by the matrix elements of the irreducible representations of the group. Therefore, the cylindrical functions of the symmetric connections $A$ are obtained by the sums of the matrix elements of the irreducible representations of the holonomies $h_I$, that is

$$f(A) = \sum_{\vec{\mu}} \sum_{j,\alpha,\beta} \xi_{\vec{\mu}}^{j\alpha\beta} \frac{R^{(j)}_{\alpha\beta}}{2} (h_1(A,\mu_1)) R^{(j_2)}_{\alpha_2\beta_2}(h_2(A,\mu_2)) R^{(j_3)}_{\alpha_3\beta_3}(h_3(A,\mu_3)) . \quad (4.2)$$

As mentioned in the beginning of Section 11 in terms of the diagonal variables, the vector constraint (3.3) is identically satisfied and thus the symmetric theory is invariant under the $SU(2)$ gauge transformation. By (4.1), on the other hand, the holonomy $h_I(A,\mu_I)$ is given by $\exp(-\frac{i}{2}\mu_I c(I)\sigma(I))$, which is not invariant if we perform a global $SU(2)$ rotation by $\sigma_I \rightarrow \sigma_I' = U_I^J \sigma_J$. Therefore, in order to have the cylindrical functions $SU(2)$-invariant, the only possibility is that all the three irreducible representations in (4.2) must be trivial (i.e. $j_1 = j_2 = j_3 = 0$) and in the trivial representation, $R^{(j=0)}(h_I(A,\mu_I))$ is simply $\exp(-\frac{i}{2}\mu_I c(I))$.

Consequently, the algebra generated by sums of products of the matrix elements of these holonomies is just the algebra of almost periodic functions of $c^I$. A typical element of the almost periodic function is written as:

$$g(c^1,c^2,c^3) = \sum_{j} \xi_j e^{i\mu_j t} c^I , \quad (4.3)$$

where $j$ runs over a finite number of integers, $\mu_j \in \mathbb{R}$ and $\xi_j \in \mathbb{C}$. As in the terminology used in the full theory, we can regard a finite number of edges labeled by $(j,I)$ as a “graph” and the function $g(c_I)$ as a cylindrical function with respect to that graph. Analogous to the space Cyl of cylindrical functions on $\mathcal{A}$ in the full theory, the vector space of the almost periodic functions is called the cylindrical functions of symmetric connections and denoted by $\text{Cyl}_S$. 

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Similarly, the momentum functions \( E(S, f) \) in the full theory is replaced by \( E(S_I, f_I) \) in the homogeneous case, which are obtained by smearing \( \tilde{E}^a \), with a constant-valued function \( f_I \) on the rectangular face \( S_I \) of the elementary cell \( V \) normal to the diagonal direction \( I \) (with respect to \( q_{ab} \)). That is

\[
E(S_I, f_I) = \int_{S_I} \Sigma_{ab}^{(I)} f_I(x) dx^a dx^b = p_I \frac{\sigma_{LI}}{V_o} A_{S_I, f_I},
\]

(4.4)

where \( \Sigma_{ab}^{(I)} = \epsilon_{abc} \bar{E}_c^i \Lambda_i I = \epsilon_{abc} \sqrt{q} p_I \epsilon_i^c \) and \( A_{S_I, f_I} \) is the area of \( S_I \) measured by \( q_{ab} \) times the orientation factor (which depends on \( f_I \)). In terms of classical geometry, \( p_I \) is related to the “physical” length of the edges and the volume of the elementary cell \( V \) via

\[
L_I = \sqrt{|p_I|} \quad \text{and} \quad V = \sqrt{|p_1 p_2 p_3|}.
\]

(4.5)

According to (3.14), the only non-vanishing Poisson brackets among the elementary functions are:

\[
\{ g(c^1, c^2, c^3), p_I \} = 4\pi \gamma G \sum_j (i \mu_j \xi_j) e^{i\mu_j K} c^K.
\]

(4.6)

The right hand side is again in \( \text{Cyl}_S \) and thus the space of the elementary variables is closed under the Poisson bracket. Note that, contrary to the full theory, the smeared momenta \( E(S_I, f_I) \) now commute with one another since they are all proportional to \( p_I \) due to homogeneity. Therefore, the triad representation in Bianchi I models does exist and this fact will be exploited in Section IV C.

### B. Representation of the Algebra of Elementary Variables

In the previous subsection, we have seen that the algebra of the elementary variables in Bianchi I models is in a perfect parallel to the case of the isotropic model studied in [6]. The elementary variables in different diagonal directions are independent of one another and each direction behaves as a copy of the isotropic case. Consequently, the result in [6] can be generalized to the Bianchi I model in the obvious way, when we construct quantum kinematics and seek a representation of the algebra of the elementary variables.

Therefore, the gravitational part of the Hilbert space for Bianchi I models is \( \mathcal{H}_{\text{grav}}^S = L^2(\mathbb{R}^3_{\text{Bohr}}, d^3\mu_{\text{Bohr}}) \), the concrete construction of which is the Cauchy completion of the space \( \text{Cyl}_S \) of almost periodic functions of \( c^I \) with respect to the inner product:

\[
\langle e^{i\vec{\mu}_I \cdot \vec{c}} | e^{i\vec{\mu}_2 \cdot \vec{c}} \rangle = \delta_{\vec{\mu}_1 \vec{\mu}_2}.
\]

(4.7)

(Here, the right hand side is the Kronecker delta, not the Dirac distribution.) Thus, the almost periodic functions \( \mathcal{N}_{\vec{\mu}}(\vec{c}) \equiv \mathcal{N}_{\mu_1, \mu_2, \mu_3}(c^1, c^2, c^3) := e^{i\vec{\mu} \cdot \vec{c}}/2 \) constitute an orthonormal basis in \( \mathcal{H}_{\text{grav}}^S \). For \( g_1 \) and \( g_2 \) in \( \text{Cyl}_S \), we have

\[
(\hat{g}_1 g_2)(\vec{c}) = g_1(\vec{c}) g_2(\vec{c})
\]

(4.8)

and by (8.14) the momentum operator is represented via

\[
\hat{p}_I = -8\pi i \gamma \ell_{\text{Pl}}^2 \frac{\partial}{\partial c^I} \quad \text{and thus} \quad (\hat{p}_I g)(\vec{c}) = 4\pi \gamma \ell_{\text{Pl}}^2 \sum_j (\xi_j \mu_{jI}) \mathcal{N}_{\vec{\mu}_j},
\]

(4.9)
where the Planck length square is defined as $\ell_{Pl}^2 = G\hbar$. The basis vectors $N_{\mu}$ are normalized eigenstates of $\hat{p}_I$. Writing $N_{\mu}(\tilde{c}) = \langle \tilde{c}|\mu \rangle$, we have

$$\hat{p}_I|\mu\rangle = 4\pi\gamma\ell_{Pl}^2|\mu\rangle \equiv p_{\mu_I}|\mu\rangle.$$  \hspace{1cm} (4.10)

Meanwhile, (4.5) also gives us the operators for the physical lengths of the edges and the volume of the cell $V$:

$$\hat{L}_I|\mu\rangle = (4\pi\gamma|\mu_I|)^{\frac{1}{2}} \ell_{Pl}|\mu\rangle \equiv L_{\mu_I}|\mu\rangle,$$  \hspace{1cm} (4.11)

$$\hat{V}|\mu\rangle = (4\pi\gamma)^{\frac{3}{2}} \sqrt{|\mu_1\mu_2\mu_3|} \ell_{Pl}^3|\mu\rangle \equiv V_{\mu}|\mu\rangle.$$  \hspace{1cm} (4.12)

### C. Inverse Triad Operators

In the case that the Hamiltonian has a matter sector minimally coupled to the gravity, when the quantum geometry is taken into account, the inverse triad operators play a key role [17]. For Bianchi I models, the inverse triad operators can be obtained by directly generalizing the result of the isotropic case in [16]. The triad coefficients $\text{sgn}(p_I)|p_I|^{-1/2}$ can be expressed as the Poisson brackets $\{c^I, L^I(\mu_I)\}$, which are then to be replaced by the commutator (divided by $i\hbar$) in quantum theory. However, as the operator corresponding to the connection does not exist in the full LQG [18, 19, 20], there is no operator $\hat{c}^I$ on $\mathcal{H}_{grav}^{S}$ corresponding to $c^I$ and we have to further re-express the Poisson bracket in terms of holonomies à la Thiemann’s trick.

On the reduced phase space, the triad coefficients can be written as:

$$\frac{\text{sgn}(p_I)}{\sqrt{|p_I|}} = \frac{1}{2\pi\gamma G \, \gamma_{\mu_I}} \text{tr} \left( \tau_I h^{(\mu_I)}_I \{ h^{(\mu_I)^{-1}}_I, L_I \} \right),$$  \hspace{1cm} (4.13)

where

$$h^{(\mu_I)}_I := \mathcal{P} \exp \left( \int_{0}^{\gamma_{\mu_I} L_I} A_a^i \tau_i \, dx^a \right) = \exp \left( \frac{\gamma_{\mu_I} c^I(\tau_I)}{2} \right).$$  \hspace{1cm} (4.14)

is the holonomy of the connection $A_a^i$ evaluated along a line of length $\gamma_{\mu_I} L_I$ (with respect to $\gamma_{ab}$) parallel to the edge of the elementary cell $V$ in the diagonal direction $I$. Note that the expression of (4.13) is independent of the choice of $\gamma_{\mu_I}$. In quantum theory, the Poisson brackets are replaced by the commutators. This leads to the inverse triad operators:

$$\left[ \frac{1}{\sqrt{|p_I|}} \right] = -\frac{i}{2\pi\gamma \ell_{Pl}^2} \text{tr} \left( \tau_I \hat{h}^{(\mu_I)}_I \{ \hat{h}^{(\mu_I)^{-1}}_I, \hat{L}_I \} \right)$$

$$= -\frac{i}{2\pi\gamma \ell_{Pl}^2} \left[ \sin \left( \frac{\gamma_{\mu_I} c^I(\tau_I)}{2} \right) \hat{L}_I \cos \left( \frac{\gamma_{\mu_I} c^I(\tau_I)}{2} \right) - \cos \left( \frac{\gamma_{\mu_I} c^I(\tau_I)}{2} \right) \hat{L}_I \sin \left( \frac{\gamma_{\mu_I} c^I(\tau_I)}{2} \right) \right].$$  \hspace{1cm} (4.15)

As in the strategy used for isotropic models, to construct inverse triad operators, there are two ambiguities, labeled by an half integer $j$ and a real number $\ell$ ($0 < \ell < 1$) [7, 21]. The general considerations in [22, 23] urge one to set $j = 1/2$. For $\ell$, a general selection criterion
is not available and $\ell = 1/2$ and $\ell = 3/4$ have been used in the literature. The difference on this choice does not affects any qualitative features and here we use $\ell = 1/2$ since it gives a simpler expression.\(^6\)

The eigenstates of the inverse triad operator are $|\vec{\mu}\rangle$ with the eigenvalues given by

\[
\left[ \frac{1}{\sqrt{|p_I|}} \right] |\vec{\mu}\rangle = \frac{1}{4\pi\gamma\ell_p^2 |p_I|} \left[ L_{\mu_1+\gamma\mu_1} - L_{\mu_1-\gamma\mu_1} \right] |\vec{\mu}\rangle, \tag{4.16}\]

where $L_{\mu_I}$ are the eigenvalues of the length operators defined in (4.11) and the equations

\[
e^{\pm i\gamma\mu_I c^1}|\mu_1,\mu_2,\mu_3\rangle = |\mu_1 \pm \gamma\mu_1,\mu_2,\mu_3\rangle, \]

\[
\cos\left(\frac{1}{2}\gamma\mu_I c^1\right)|\mu_1,\mu_2,\mu_3\rangle = \frac{1}{2} \left( |\mu_1+\gamma\mu_1,\mu_2,\mu_3\rangle + |\mu_1-\gamma\mu_1,\mu_2,\mu_3\rangle \right), \]

\[
\sin\left(\frac{1}{2}\gamma\mu_I c^1\right)|\mu_1,\mu_2,\mu_3\rangle = \frac{1}{2i} \left( |\mu_1+\gamma\mu_1,\mu_2,\mu_3\rangle - |\mu_1-\gamma\mu_1,\mu_2,\mu_3\rangle \right) \tag{4.17}\]

as well as the corresponding ones for $c^2$ and $c^3$ are used. While the choice of $\gamma\mu_I$ gives no difference in classical level, it changes the eigenvalues of the inverse triad operators. The difference due to $\gamma\mu_I$ is negligible when the operators act on the states $|\vec{\mu}\rangle$ with $|\mu_I| \gg \gamma\mu_I$ and becomes significant when the values of $\mu_I$ are comparable to $\gamma\mu_I$. In $\gamma\mu$-scheme, we will impose $\gamma\mu_I = k \equiv \sqrt{3}/2$ as the imprint of the fundamental discreteness in the full theory (see Section [VIA]), while in $\vec{\mu}$-scheme, the inverse triad operators are redefined in a refined way such that $\gamma\mu_I$ are replaced by $\vec{\mu}_I$, which vary adaptively on different states $|\vec{\mu}\rangle$ (see Section [VII B]).

Since the inverse triad operator is diagonal with real eigenvalues in the basis of $|\vec{\mu}\rangle$, it is self-adjoint in $H^S_{grav}$. It can also be shown that the inverse triad operator commutes with $\hat{p}_I$ despite the presence of $c^I$ in (1.15). A key property of the inverse triad operators is that they are all bounded above. At the value $\mu_I = \pm \gamma\mu_I$, the upper bound is obtained:

\[
|p_I|^{\frac{1}{2}} = (2\pi\gamma)^{-1/2} \ell_{Pl}^{-1}. \tag{4.18}\]

The fact that the eigenvalue of $1/\sqrt{|p_I|}$ goes to zero (instead of infinity) when $\mu_I \to 0$ commands the matter part of the Hamiltonian constraint $\hat{C}_{matter}(\vec{\mu})$ to annihilate $\Psi(\vec{\mu}, \phi)$ for $\mu_1 = 0, \mu_2 = 0$ or $\mu_3 = 0$. This is an important condition that accounts for the resolution of the singularity (see the remark in Section [VII C]). (More physical implications from the finiteness of the inverse triad operator are discussed in detail in [6].)

V. DYNAMICS: HAMILTONIAN CONSTRAINT ($\gamma\mu$-SCHEME)

To study the quantum dynamics, we need to obtain the Hamiltonian constraint in the quantum theory. We follow the same procedures used in [1, 2, 6] to construct the gravitational constraint operator in $\gamma\mu$-scheme. The self-adjointness of the gravitational constraint operator and its WDW limit are also discussed. This section focuses only on the gravitational part of the constraint operator. The total Hamiltonian including the matter sector and a more complete study of the analytical issues will be explored in Section VII. The improved dynamics in $\vec{\mu}$-scheme is left in Section [VIII].

\[^6\] Note that $\ell = 3/4$ was used in [1] while $\ell = 1/2$ was used in [8].
A. Gravitational Constraint Operator

In the classical theory, the Hamiltonian constraint in the Bianchi I model is given by (3.22). However, since the corresponding operator \( \hat{c}' \) does not exist, we cannot directly use the Hamiltonian of this form but should recast it in terms of holonomies of the symmetric connections. To bring out the close similarity of the regularization procedure to that in the full theory, we start from the expression of the classical constraint in the full theory, which is

\[
C_{\text{grav}} := \int_{\mathcal{V}} d^3 N e^{-1} \left( \epsilon_{ijk} F_{ab}^i \tilde{E}^{aj} \tilde{E}^{bk} - 2(1 + \gamma^2) K_{[a}^i K_{b]}^j \tilde{E}^{a}_{,i} \tilde{E}^{b}_{,j} \right)
\]

\[
= -\gamma^{-2} \int_{\mathcal{V}} d^3 x N \epsilon_{ijk} F_{ab}^i e^{-1} \tilde{E}^{aj} \tilde{E}^{bk},
\]  

(5.1)

where \( e := \sqrt{|\det \tilde{E}|} \, \text{sgn}(\det \tilde{E}) = \text{sgn}(p_1 p_2 p_3) \sqrt{|p_1 p_2 p_3|} \) and the integral is restricted to the elementary cell \( \mathcal{V} \) (of volume \( V_o = L_1 L_2 L_3 \) with respect to \( q_{ab} \)). In the second line of (5.1), we exploit the fact that for spatially flat models, the two terms in the first line are proportional to each other (because \( -\gamma K_{a}^i = A_a^i \) and \( F_{ab}^i = \epsilon_{ijk} A_a^i A_b^j \) when the spatial slice is flat). Because of homogeneity, the lapse \( N \) can be assumed to be constant and from now on we set it to one.

To construct the Hamiltonian constraint operator, we first follow the standard strategy used in gauge theories to express the curvature component \( F_{ab}^i \) in terms of holonomies. Given a small rectangular surface \( \alpha_{IJ} \) parallel to the face of the cell \( \mathcal{V} \) in the \( I-J \) plane (the two edges of \( \alpha_{IJ} \) are of lengths \( q_{I} \, L_I \) and \( q_{J} \, L_J \) with respect to \( q_{ab} \)), the “ab component” of the curvature can be written as

\[
F_{ab}^i \tau_i = \sum_{I \neq J} q_{a}^I q_{b}^J \left( \frac{h_{(\mu)_{IJ}}}{q_{I} q_{J} L_I L_J} - 1 \right) \mathcal{O}(c^3 \mu) ,
\]

(5.2)

The holonomy around the perimeter of \( \alpha_{IJ} \) is:

\[
h_{(\mu)_{IJ}} = h_{1}^{(\mu)} h_{J}^{(\mu)} (h_{I}^{(\mu)})^{-1} (h_{J}^{(\mu)})^{-1},
\]

(5.3)

where the holonomy along the individual edges \( h_{1}^{(\mu)} \) is given by (4.14).

Next, following the close similarity of the regularization procedure used in the full theory [24, 25, 26], we express the triad term \( \epsilon_{ijk} e^{-1} \tilde{E}^{aj} \tilde{E}^{bk} \) in terms of holonomies and the Poisson brackets of the holonomy and the volume function. In the symmetry reduced phase space, this is done as:

\[
\tau_i \epsilon_{ijk} e^{-1} \tilde{E}^{aj} \tilde{E}^{bk} = -\frac{2}{8 \pi^3 G} \sum_{K} \frac{\text{sgn}(p_1 p_2 p_3)}{q_{K} q_{L} L_K} \epsilon_{abc} \omega_c K h_{K}^{(\mu K)} \left\{ h_{K}^{(\mu K)}^{-1}, V \right\},
\]

(5.4)

where \( V = L_1 L_2 L_3 = \sqrt{|p_1 p_2 p_3|} \). Note that (5.4) is exact, while (5.2) depends on the choice of \( q_{\mu} \) (“\( \mu \)-ambiguity”).

Taking (5.2) and (5.4) into (5.1), we have

\[
C_{\text{grav}} = -\frac{4}{8 \pi^3 G} \sum_{IJK} \frac{\text{sgn}(p_1 p_2 p_3)}{q_{I} q_{J} q_{K}} \epsilon_{IJK} \text{tr} \left( h_{1}^{(\mu I)} h_{J}^{(\mu J)} h_{I}^{(\mu K)} h_{J}^{(\mu J)} h_{I}^{(\mu K)} \left\{ h_{K}^{(\mu K)}^{-1}, V \right\} \right) + \mathcal{O}(c^3 \mu),
\]

(5.5)
where the term proportional to the identity inside the parenthesis in (5.2) is dropped out because of the trace and because the equations $\epsilon^{abc} \omega_a \omega_b \omega_c K = \sqrt{\eta} \epsilon^{JK} \text{ and } \int_V d^3x \sqrt{\eta} = V_o$ are used. Note that the limit $\mu_I \to 0$ in (5.5) exists and it precisely equals the classical counterpart $C_{grav}$ in (3.22). However, this limit is physically fictitious and only makes sense mathematically. Since $\hat{c}$ is not well-defined in $\mathcal{H}_{grav}$, the “continuum limit” $\mu_I \to 0$ fails to exist and thus we cannot remove the regulator in the quantum geometry of the reduced model. (In the full theory, on the contrary, diffeomorphism invariance ensures the insensitivity to the regularization procedure [24, 25, 26]. The dependence on the regulator is traced back to the assumption of homogeneity.)

Since there is no natural way to express the constraint exactly in terms of the elementary variables, the limiting procedure is essential. To faithfully convey the underlining geometry of the full theory, we keep $\mu_I$ explicitly and treat it as the “regulator”, which reflects the “fundamental discreteness” of the full theory as an imprint on the reduced theory. (The appropriate value of $\mu_I$ is to be determined soon.) The resulting regulated constraint is:

$$
\hat{C}_{grav,o}^{(\mu)} = \frac{4i \text{ sgn}(p_1 p_2 p_3)}{8\pi \gamma^3 \ell_P^2 \gamma_{12}^3} \sum_{IJK} \epsilon_{IJK} \text{tr} \left( \hat{h}_I^{(\mu)} \hat{h}_J^{(\mu)} \hat{h}_K^{(\mu)} \hat{h}_I^{(\mu-1)} \hat{h}_J^{(\mu-1)} \hat{h}_K^{(\mu-1)} \right) \hat{V} 
$$

$$
= \frac{i \text{ sgn}(p_1 p_2 p_3)}{\pi \gamma^3 \ell_P^2 \gamma_{12}^3} \left\{ \sin(\mu_1 c^1) \sin(\mu_2 c^2) \left( \sin(\mu_3 c^3) \hat{V} \cos(\mu_3 c^3) - \cos(\mu_3 c^3) \hat{V} \sin(\mu_3 c^3) \right) 
+ \text{cyclic terms} \right\},
$$

(5.6)

where “cyclic terms” denote the same expression as the term(s) written explicitly inside the curly bracket but with the cyclic index replacements $(1 \to 2, 2 \to 3, 3 \to 1)$. (The subscript “o” used for $\hat{C}_{grav,o}^{(\mu)}$ is to indicate that the ordering ambiguity of quantization has not been taken care of and thus $\hat{C}_{grav,o}^{(\mu)}$ is not self-adjoint.) The operator $\hat{C}_{grav,o}^{(\mu)}$ acting on the eigenstates of $\hat{p}_I$ gives

$$
\hat{C}_{grav,o}^{(\mu)} |\mu_1, \mu_2, \mu_3\rangle = \frac{1}{8\pi \gamma^3 \ell_P^2 \gamma_{12}^3} \times \left\{ |V_{\mu_1, \mu_2, \mu_3} - V_{\mu_1, \mu_2, \mu_3 - \mu_3}| \left( |\mu_1 + 2 \mu_1, \mu_2 + 2 \mu_2, \mu_3\rangle - |\mu_1 - 2 \mu_1, \mu_2 + 2 \mu_2, \mu_3\rangle \right) 
- |\mu_1 + 2 \mu_1, \mu_2 - 2 \mu_2, \mu_3\rangle + |\mu_1 - 2 \mu_1, \mu_2 - 2 \mu_2, \mu_3\rangle \right) 
+ \text{cyclic terms},
$$

(5.7)

where (4.17) is used. Regarded as a state in the connection representation, (every element of) the holonomy $h_I^{(\mu)}$ is an eigenstate of the area operator $\hat{a}_I = [p_I]$:

$$
\hat{a} h_I^{(\mu)} (c) = (4\pi \gamma \mu_I \ell_P^2) h_I^{(\mu)} (c).
$$

(5.8)

Following the same strategy (\mu-scheme) in [27, 28, 29], we demand this eigenvalue to be be $\Delta = 2\sqrt{3} \pi \gamma \ell_P^2$, the area gap of the full theory. This yields $\mu_I = k := \Delta / (4\pi \gamma \ell_P^2) = \sqrt{3}/2$ and fixes the “\mu-ambiguity”.

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B. Self-Adjointness and the WDW Limit

In order to construct the physical sector with the physical inner product (which will be done in Section VII), it is advantageous to have the Hamiltonian constraint self-adjoint. Note that (5.6) is not self-adjoint. This happens simply because of the factor ordering ambiguities common in quantum mechanics. There are two natural ways to resolve the ordering problems. The first is to take the self-adjoint part of (5.6):

$$\hat{C}^{(\gamma)}_{\text{grav}} = \frac{1}{2} \left[ \hat{C}^{(\gamma)}_{\text{grav}, o} + \hat{C}^{(\gamma)}_{\text{grav}, o} \dagger \right].$$  \hspace{1cm} (5.9)

The second is the nature re-ordering adopted in [1], in which we “re-distribute” the $\sin(\mu_c)$ terms to get the following self-adjoint constraint:

$$\hat{C}^{(\mu)}_{\text{grav}} = \frac{4\pi \text{sgn}(p_1 p_2 p_3)}{8\pi^3 \ell^{-2}_p} \hat{q}_{\mu_1} \hat{q}_{\mu_2} \hat{q}_{\mu_3}$$

$$\times \left\{ \sin(\mu_1 c) \left( \sin\left(\frac{\mu_3 c^3}{2}\right) \hat{V} \cos\left(\frac{\mu_3 c^3}{2}\right) - \cos\left(\frac{\mu_3 c^3}{2}\right) \hat{V} \sin\left(\frac{\mu_3 c^3}{2}\right) \right) \sin(\mu_2 c^2) 
+ \sin(\mu_2 c^2) \left( \sin\left(\frac{\mu_3 c^3}{2}\right) \hat{V} \cos\left(\frac{\mu_3 c^3}{2}\right) - \cos\left(\frac{\mu_3 c^3}{2}\right) \hat{V} \sin\left(\frac{\mu_3 c^3}{2}\right) \right) \sin(\mu_1 c) \right\}. \hspace{1cm} (5.10)$$

When acting on the eigenstates of $\hat{p}_I$, $\hat{C}^{(\mu)}_{\text{grav}}$ gives

$$\hat{C}^{(\gamma)}_{\text{grav}} |_{\gamma} = \frac{1}{16\pi^3 \ell^{-2}_p} \hat{q}_{\mu_1} \hat{q}_{\mu_2} \hat{q}_{\mu_3}$$

$$\times \left\{ \left| V_{\mu_1 + 2\mu_1, \mu_2 + 2\mu_2, \mu_3 + 2\mu_3} - V_{\mu_1 + 2\mu_1, \mu_2 + 2\mu_2, \mu_3 - 2\mu_3} \right| + \left| V_{\mu_1, \mu_2, \mu_3 + 2\mu_3} - V_{\mu_1, \mu_2, \mu_3 - 2\mu_3} \right| \right\} |_{\gamma}$$

$$= 1$$

$$\times \left\{ \left| V_{\mu_1 + 2\mu_1, \mu_2 + 2\mu_2, \mu_3 + 2\mu_3} - V_{\mu_1 + 2\mu_1, \mu_2 + 2\mu_2, \mu_3 - 2\mu_3} \right| + \left| V_{\mu_1, \mu_2, \mu_3 + 2\mu_3} - V_{\mu_1, \mu_2, \mu_3 - 2\mu_3} \right| \right\} |_{\gamma}$$

$$\times \left\{ \left| V_{\mu_1 + 2\mu_1, \mu_2 + 2\mu_2, \mu_3 + 2\mu_3} - V_{\mu_1 + 2\mu_1, \mu_2 + 2\mu_2, \mu_3 - 2\mu_3} \right| + \left| V_{\mu_1, \mu_2, \mu_3 + 2\mu_3} - V_{\mu_1, \mu_2, \mu_3 - 2\mu_3} \right| \right\} |_{\gamma}$$

$$+ \text{cyclic terms} \}. \hspace{1cm} (5.11)$$

and $\hat{C}^{(\gamma)}_{\text{grav}}$ gives

$$\hat{C}^{(\mu)}_{\text{grav}} |_{\gamma} = \frac{1}{16\pi^3 \ell^{-2}_p} \hat{q}_{\mu_1} \hat{q}_{\mu_2} \hat{q}_{\mu_3}$$

$$\times \left\{ \left| V_{\mu_1 + 2\mu_1, \mu_2 + 2\mu_2, \mu_3 + 2\mu_3} - V_{\mu_1 + 2\mu_1, \mu_2 + 2\mu_2, \mu_3 - 2\mu_3} \right| + \left| V_{\mu_1, \mu_2, \mu_3 + 2\mu_3} - V_{\mu_1, \mu_2, \mu_3 - 2\mu_3} \right| \right\} |_{\gamma}$$

$$- \left\{ \left| V_{\mu_1 + 2\mu_1, \mu_2 + 2\mu_2, \mu_3 + 2\mu_3} - V_{\mu_1 + 2\mu_1, \mu_2 + 2\mu_2, \mu_3 - 2\mu_3} \right| + \left| V_{\mu_1, \mu_2, \mu_3 + 2\mu_3} - V_{\mu_1, \mu_2, \mu_3 - 2\mu_3} \right| \right\} |_{\gamma}$$

$$+ \text{cyclic terms} \}. \hspace{1cm} (5.12)$$
In this paper, we choose the second method of symmetrization, since \( \hat{C}_{\text{grav}}^{(\mu)} \) has certain qualities better than \( \hat{C}_{\text{grav}}^{(\mu)'} \). In particular, in the isotropic cases, \( \hat{C}_{\text{grav}}^{(\mu)} \) gives positive definite \( \Theta \) (to be defined later), which is a pleasing feature when the physical sector is constructed. In the anisotropic Bianchi I model, the positive definiteness of \( \Theta \) no longer holds; nevertheless, choosing \( \hat{C}_{\text{grav}}^{(\mu)} \) enables us to generalize the isotropic results in an obvious way.

The Hamiltonian constraint equation differs markedly from the WDW equation of geometrodynamics in the Planck regime because it crucially exploits the discreteness underlying quantum geometry. In the continuum limit \( \mu_I \rightarrow 0 \) (although physically fictitious), one expect that the LQC constraint equation will reduce to the WDW equation. According to the analysis in \([1]\) (and more details in \([6]\)), we can follow the argument therein and conclude that the gravitational part of the Hamiltonian operators reduces to:

\[
\hat{C}_{\text{grav},o}^{(\mu)} \Psi(\vec{p}) \approx 128\pi^2\ell_P^4 \left\{ \frac{\text{sgn}(p_1 p_2)}{\sqrt{|p_3|}} \sqrt{|p_1 p_2|} \frac{\partial^2}{\partial p_1 \partial p_2} + \text{cyclic terms} \right\} \Psi(\vec{p})
\]

\[=: \hat{\tilde{C}}_{\text{grav},o}^{\text{WDW}} \Psi(\vec{p}), \quad (5.13)\]

\[
\hat{C}_{\text{grav}}^{(\mu)'} \Psi(\vec{p}) \approx 64\pi^2\ell_P^4 \left\{ \frac{\text{sgn}(p_1 p_2)}{\sqrt{|p_3|}} \left( \sqrt{|p_1 p_2|} \frac{\partial^2}{\partial p_1 \partial p_2} + \frac{\partial^2}{\partial p_1 \partial p_2} \sqrt{|p_1 p_2|} \right) + \text{cyclic terms} \right\} \Psi(\vec{p})
\]

\[=: \hat{\tilde{C}}_{\text{grav}}^{\text{WDW}} \Psi(\vec{p}), \quad (5.14)\]

\[
\hat{C}_{\text{grav}}^{(\mu)} \Psi(\vec{p}) \approx 64\pi^2\ell_P^4 \left\{ \frac{\text{sgn}(p_1 p_2)}{\sqrt{|p_3|}} \left( \frac{\partial}{\partial p_2} \sqrt{|p_1 p_2|} \frac{\partial}{\partial p_1} + \frac{\partial}{\partial p_1} \sqrt{|p_1 p_2|} \frac{\partial}{\partial p_2} \right) + \text{cyclic terms} \right\} \Psi(\vec{p})
\]

\[=: \hat{\tilde{C}}_{\text{grav}}^{\text{WDW}} \Psi(\vec{p}). \quad (5.15)\]

In the above approximations, \( \approx \) stands for equality modulo terms of the order \( \mathcal{O}(\mu_I) \) (where \( \mu_I := 4\pi \gamma \ell_P^2 \mu_I \)). That is, in the limit when the characteristic scale is much greater than that associated with the area gap (i.e. \( |p_I| \gg \mu_I \) or \( |\mu_I| \gg \mu_I \)), quantum geometry effects can be neglected and the LQC difference operators reduce to the WDW differential operators. The different ordering factors give rise to different WDW limits. In particular, \( \hat{C}_{\text{grav}}^{(\mu)'} \) and \( \hat{C}_{\text{grav}}^{(\mu)} \) differ only by a factor ordering:

\[
(\hat{C}_{\text{grav}}^{(\mu)'} - \hat{C}_{\text{grav}}^{(\mu)}) \Psi(\vec{p}) = \frac{48\pi^2\ell_P^4}{\sqrt{|p_1 p_2 p_3|}} \left( \text{sgn}(p_1 p_2) + \text{sgn}(p_1 p_3) + \text{sgn}(p_2 p_3) \right) \Psi(\vec{p}). \quad (5.16)
\]

The difference is negligible for large (volume) scales. The operator \( \hat{\tilde{C}}_{\text{grav}}^{\text{WDW}} \) will be used extensively in Section \([VI]\).

**Note:** The results obtained in this section can be formally “translated” for the isotropic case by inspection. The translation and the related issues of isotropy reduction from anisotropic models in \( \gamma\mu \)-scheme are remarked in Appendix \([B.1]\). \( \square \)

**VI. WHEELER-DEWITT (WDW) THEORY**

In this section, we make a digression to study and construct the WDW quantum theory in the *connection dynamics*. This construction will serve two purposes: first, it will introduce
the key notions for constructing the physical space and enable us to generalized these notions
heuristically for the completion of the program in LQC; second, we will be able to compare
and contrast the results of the WDW and LQC theories, thereby extracting out the essential
ingredient given by the quantum geometry. In particular, the WDW theory does not
resolve the classical singularity but the semi-classical (coherent) states in the WDW theory can be
used to build up the initial states at late times in LQC theory.

A. Emergent Time and the General Solutions

Recall that the classical Hamiltonian constraint in terms of the variables \( c^I \) and \( p_I \) is
given by (3.22); that is

\[
C_\phi = -C_{\text{grav}} \Rightarrow 8\pi G |p_1 p_2 p_3|^{-1/2} \phi^2 = \frac{2}{\gamma^2} \left( \frac{\text{sgn}(p_1 p_2)}{\sqrt{|p_3|}} c^1 c^2 \sqrt{|p_1 p_2|} + \text{cyclic terms} \right).
\]

(6.1)

In WDW theory, we have the kinematic Hilbert space \( \mathcal{H}_{\text{kin}}^{\text{WDW}} = L^2(\mathbb{R}^2, dp d\phi) \). The operators \( \hat{p}_I \) and \( \hat{\phi} \) act as multiplications while \( \hat{c}^I \) and \( \hat{p}_\phi \) act as differential operators, represented as:

\[
\hat{c}^I \Psi = i\hbar 8\pi \gamma G \frac{\partial \Psi}{\partial p_I} \quad \text{and} \quad \hat{p}_\phi \Psi = -i\hbar \frac{\partial \Psi}{\partial \phi}.
\]

(6.2)

To write down the quantum constraint operator, we have to make a choice of the factor
ordering. Since our purpose is to compare the WDW theory with LQC, it is most con-
venient to use the same factor ordering that comes from the cont inuum limit of the LQC
constraint. Therefore, we chose \( \hat{C}_{\text{grav}}^{\text{WDW}} \) defined in (5.15) as the gravitational part of the
WDW Hamiltonian constraint. The total WDW Hamiltonian constraint then reads as

\[
\frac{\partial^2 \Psi}{\partial \phi^2} = 8\pi G [\mathcal{B}(\vec{\mu})]^{-1} \left\{ \frac{\text{sgn}(\mu_1 \mu_2)}{\sqrt{|\mu_3|}} \left( \frac{\partial}{\partial \mu_2} \sqrt{|\mu_1 \mu_2|} \frac{\partial}{\partial \mu_1} + \frac{\partial}{\partial \mu_1} \sqrt{|\mu_1 \mu_2|} \frac{\partial}{\partial \mu_2} \right) + \text{cyclic terms} \right\} \Psi \\
= - (\Theta_3(\mu_1, \mu_2) + \Theta_2(\mu_1, \mu_3) + \Theta_1(\mu_2, \mu_3)) \Psi =: -\Theta(\vec{\mu}) \Psi,
\]

(6.3)

where we define \( p_I = 4\pi \gamma \ell_p^2 \mu_I \) and \( \mathcal{B}(\vec{\mu}) := |\mu_1 \mu_2 \mu_3|^{-1/2} \). The WDW equation now has the
same form as the Klein-Gordon equation, with \( \phi \) playing the role of time and \( \Theta \) of the spatial
Laplacian. Therefore, the form of the Hamiltonian constraint in the WDW theory suggests
that \( \phi \) can be interpreted as emergent time. Unlike the isotropic case, however, \( \Theta \) is not
elliptic and hence not positive definite. Fortunately, this problem can be easily overcome.
We will see soon that the subspace of negative eigenvalues of \( \Theta \) is actually non-physical and
it turns out only \( \Theta_+ \), the projection on the positive spectrum of \( \Theta \), does matter.

Note that if \( \Psi(\vec{\mu}, \phi) \) is a solution of (6.3), so is \( \Pi_I \Psi(\vec{\mu}, \phi) \) (where \( \Pi_I \) are the orientation
reversal operators, which flip \( \mu_I \) to \( -\mu_I \) for \( I = 1, 2, 3 \)) since \( \Theta \) commutes with \( \Pi_I \). Because
the standard WDW theory deals with geometry, it is completely insensitive to the orientation
of the triad and \( \Pi_I \) should be considered as large gauge transformations. Furthermore, \( \Pi_3^2 = 1 \) and there are only two eigenspaces of \( \Pi_I \), one of which is the symmetric sector and
the other anti-symmetric. Therefore, it is natural to work with the symmetric sector. Thus,
the physical Hilbert space will consist of the suitably regular solutions \( \Psi(\mu, \phi) \) to (6.3) which
are symmetric under \( \mu_I \to -\mu_I \) for \( I = 1, 2, 3 \).
To obtain the general solution of (6.3), we first note that the operator enclosed by the curly bracket in (6.3) is self-adjoint on $L^2_S(\mathbb{R}^3, d^3\vec{\mu})$, the invariant subspace of $L^2(\mathbb{R}^3, d^3\vec{\mu})$ under $\Pi_{i=1,2,3}$. Therefore, $\Theta$ (and $\Theta_f$ as well) is self-adjoint on $L^2_S(\mathbb{R}^3, \mathcal{B}(\vec{\mu}) d^3\vec{\mu})$. It is easy to verify that the eigenfunctions of $\Theta$ can be labeled by $\vec{k} \in \mathbb{R}^3$:

$$e_{\vec{k}}(\vec{\mu}) = \frac{1}{(4\pi)^3} |\mu_1\mu_2\mu_3|^\frac{1}{2} e^{ik_1\ln|\mu_1|} e^{ik_2\ln|\mu_2|} e^{ik_3\ln|\mu_3|}. \quad (6.4)$$

The corresponding eigenvalues are given by

$$\Theta e_{\vec{k}}(\vec{\mu}) = \omega^2(\vec{k}) e_{\vec{k}}(\vec{\mu}) \quad \text{with} \quad \omega^2(\vec{k}) = 16\pi G \left( k_1 k_2 + k_1 k_3 + k_2 k_3 + \frac{3}{16} \right) \quad (6.5)$$

(where the factor $3/16$ is an artifact of the factor ordering choice). The eigenfunctions satisfy the orthonormality relation:

$$\int d^3\mu \mathcal{B}(\vec{\mu}) \overline{e_{\vec{k}}}(\vec{\mu}) \overline{e_{\vec{k}'}}(\vec{\mu}) = \delta^3(\vec{k}, \vec{k}'), \quad (6.6)$$

(where the right hand side is the standard Dirac distribution) and the completeness relation:

$$\int d^3\mu \mathcal{B}(\vec{\mu}) \overline{e_{\vec{k}}}(\vec{\mu}) \Psi(\vec{\mu}) = 0 \quad \text{for all} \ \vec{k}, \ \text{iff} \ \Psi(\vec{\mu}) = 0 \quad (6.7)$$

for any $\Psi(\vec{\mu}) \in L^2_S(\mathbb{R}^3, \mathcal{B}(\vec{\mu}) d^3\vec{\mu})$.

Unlike the case of isotropic model, however, $\Theta$ is not positive definite on $\Psi(\vec{\mu}) \in L^2_S(\mathbb{R}^3, \mathcal{B}(\vec{\mu}) d^3\vec{\mu})$ and $\omega^2$ could be negative. If $\omega^2 < 0$, the frequency has imaginary part and the corresponding plane wave solution to (6.3) blows up in the far future ($\phi \rightarrow \infty$) or far past ($\phi \rightarrow -\infty$); therefore, the modes associated with negative $\omega^2$ should be discarded and only those with $\omega^2 > 0$ are allowed. The relevant space is the “positive” subspace $L^2_S(\mathbb{R}^3, \mathcal{B}(\vec{\mu}) d^3\vec{\mu}; \omega^2 > 0)$ and what matters is just the operator $\Theta_+$, obtained by projecting the action of $\Theta$ to the positive eigenspace in its spectral decomposition.\(^7\)

With the eigenfunctions in hand, we can express the “general” solution to (6.3) as

$$\Psi(\vec{\mu}, \phi) = \int_{\omega^2(\vec{k}) > 0} d^3k \left( \bar{\Psi}_+(\vec{k}) e^{i\omega\phi} + \bar{\Psi}_-(\vec{k}) \overline{e_{\vec{k}}}(\vec{\mu}) e^{-i\omega\phi} \right) \quad (6.9)$$

---

\(^7\) The physical condition $\omega^2 > 0$ is reminiscent of the constraint (2.7) on the classical solution parameters $\kappa_1$, $\kappa_2$, $\kappa_3$ and $\kappa_\phi$, which leads to $\kappa_\phi^2 = 2(\kappa_1 \kappa_2 + \kappa_1 \kappa_3 + \kappa_2 \kappa_3)$. If we have the identification: $k_{1,2,3} = K \kappa_{1,2,3}$, then the frequency gives

$$\omega^2(\vec{k}) = 8\pi G \left( K^2 \kappa_\phi^2 + \frac{3}{8} \right) \approx 8\pi G K^2 \kappa_\phi^2 \equiv \frac{\nu_\phi^2}{\hbar^2} > 0, \quad (6.8)$$

(where the approximation is valid when $p_\phi \gg \hbar \sqrt{G}$ or equivalently $K \kappa_\phi \gg 1$). This shows that the physical condition $\omega^2 > 0$ simply means $p_\phi$ is real. For a semi-classical state, the identification $k_{1,2,3} = K \kappa_{1,2,3}$ is sensible, since its Fourier transformed function $\bar{\Psi}_\pm(\vec{k})$ (to be defined below) is sharply peaked at $k_{1,2,3} = K \kappa_{1,2,3}$. (See Section [VI.C] for more details.)
for some $\tilde{\Psi}_\pm(\vec{k})$ in $L^2(\mathbb{R}^3, d^3k)$. Following the terminology used in the Klein-Gordon theory, if $\tilde{\Psi}_\pm(\vec{k})$ has support in the region of positive $k_I$, we call the solution “incoming” (or “expanding”) in the direction $I$, while if it has support of negative $k_I$, it is said to be “outgoing” (or “contracting”).

8 If $\tilde{\Psi}_+/-(\vec{k})$ vanishes, the solution is said to be negative/positive frequency. Thus, every solution (6.9) admits a natural decomposition into the positive and negative frequency parts. The positive (respectively negative) frequency solutions satisfy the first order (in $\phi$) equation which can be regarded as the square-root of (6.3):

$$\frac{\partial \Psi_\pm}{\partial \phi} = \pm i \sqrt{\Theta_+} \Psi_\pm,$$

where $\sqrt{\Theta_+}$ is the square-root of the positive self-adjoint operator $\Theta_+$ defined via spectral decomposition on $L^2(\mathbb{R}^3, \mathcal{B}(\vec{\mu}) d^3\mu; \omega^2 > 0)$. Therefore, a general “initial” function $\Psi_\pm(\vec{\mu}, \phi_o) = f_\pm(\vec{\mu}) \in L^2(\mathbb{R}^3, \mathcal{B}(\vec{\mu}) d^3\mu; \omega^2 > 0)$ at $\phi = \phi_o$ can be “evolved” to a solution of (6.3) by:

$$\Psi_\pm(\vec{\mu}, \phi) = e^{\pm i \sqrt{\Theta_+} (\phi - \phi_o)} \Psi_\pm(\vec{\mu}, \phi_o).$$

### B. The Physical Sector

To endow the space of the WDW solutions with a Hilbert space structure, we follow the same strategy of [1]. The idea is to introduce the operators corresponding to a complete set of Dirac observables and select the required inner product by demanding that those Dirac operators all be self-adjoint. In the classical theory, a complete set is given by $\hat{p}_\phi$ and $\hat{\mu}_I|_{\phi_o}$ ($\vec{\mu}$ at some particular instant $\phi = \phi_o$), since the set of these uniquely specifies a classical solution and thus represents a point in the classical phase space. In WDW theory, given a (symmetric) solution $\Psi(\vec{\mu}, \phi)$, since $\hat{p}_\phi$ commutes with $\Theta$,

$$\hat{p}_\phi \Psi(\vec{\mu}, \phi) := -i\hbar \frac{\partial \Psi}{\partial \phi}$$

is again a (symmetric) solution to the WDW equation. So, we can just retain this definition of $\hat{p}_\phi$ from $\mathcal{H}_{\text{kin}}^{\text{WDW}}$. On the other hand, (6.11) enables us to define the Dirac observables $\mu_I|_{\phi_o}$. For a given (symmetric) solution $\Psi(\vec{\mu}, \phi)$, we decompose it into the positive and negative parts $\Psi_\pm(\vec{\mu}, \phi)$, freeze them at $\phi = \phi_o$, multiply them by $|\mu_I|$ and evolve each of them by (6.11). That is

$$\mu_I|_{\phi_o} \Psi(\vec{\mu}, \phi) := e^{i \sqrt{\Theta_+} (\phi - \phi_o)} |\mu_I| \Psi_+(\vec{\mu}, \phi_o) + e^{-i \sqrt{\Theta_+} (\phi - \phi_o)} |\mu_I| \Psi_-(\vec{\mu}, \phi_o).$$

The result is again a (symmetric) solution to (6.3).

---

8 The name of “expanding/contracting” makes sense for semi-classical solutions, for which $k_I$ is supported mainly in the vicinity of $K_\kappa_I$ as mentioned in the previous footnote. According to (2.9), if $\kappa_I$ is positive/negative (and $\kappa_\phi > 0$), the scale factor $a_I$ in the direction $I$ is expanding/contracting with respect to $\phi$. [Note: The nomenclature adopted here is opposite to that in [1], due to the minus sign used in the equation there: $p^{\star}_\phi = -\hbar \sqrt{3/16\pi G k^*}$, which, in the anisotropic notations, gives rise to an extra minus sign for the relation between $\kappa_\phi$ and $p^{\star}_\phi$ in (6.20).]
Note that both \( \hat{p}_\phi \) and \( \hat{\mu}_I |_{\phi_o} \) preserve the positive and negative frequency sectors and hence we have super-selection between these two sectors. In quantum theory, we can restrict ourselves on one of them. From now on, we will focus on the positive frequency sector and thus drop the suffix + for \( \Psi \).

Every WDW solution is uniquely determined by its initial condition \( \Psi(\vec{\mu},\phi_o) \) and the Dirac observables have the actions on the initial state:

\[
\hat{\mu}_I |_{\phi_o} \Psi(\vec{\mu},\phi_o) = |\mu_I| \Psi(\vec{\mu},\phi_o) \quad \text{and} \quad \hat{p}_\phi \Psi(\vec{\mu},\phi_o) = \hbar \sqrt{\Theta} \Psi(\vec{\mu},\phi_o). \quad (6.14)
\]

The unique (up to an overall scaling) inner product which makes these Dirac observables self-adjoint is therefore given by

\[
\langle \Psi_1 | \Psi_2 \rangle_{\text{phy}} = \int d^3 B(\vec{\mu}) \tilde{\Psi}_1(\vec{\mu},\phi_o) \Psi_2(\vec{\mu},\phi_o). \quad (6.15)
\]

(Note that the inner product is conserved, i.e., independent of the choice of the initial instant \( \phi_o \).) As a result, the physical Hilbert space \( H_{\text{phy}}^{\text{WDW}} \) is the space of wave functions \( \Psi(\vec{\mu},\phi) \) which are symmetric under \( \mu_I \to -\mu_I \) and have finite norm by (6.15). The representation of the complete Dirac observables on \( H_{\text{phy}}^{\text{WDW}} \) is given by

\[
\hat{\mu}_I |_{\phi_o} \Psi(\vec{\mu},\phi) = e^{i \sqrt{\Theta} (\phi - \phi_o)} |\mu_I| \Psi(\vec{\mu},\phi_o) \quad \text{and} \quad \hat{p}_\phi \Psi(\vec{\mu},\phi) = \hbar \sqrt{\Theta} \Psi(\vec{\mu},\phi). \quad (6.16)
\]

With the Dirac operators as well as the physical inner product in hand, we are able to calculate the expectation and uncertainty of the physical observables for a given physical state and thereby to extract the physics in WDW theory.

The same representation of the algebra of Dirac observables can be obtained by the more systematic group averaging method \([30, 31, 32, 33, 34]\), as has been done for the isotropic model in \([1]\). There may be some complications in anisotropic cases and we defer this issue to future study.

C. The Semi-Classical (Coherent) States

With the physical Hilbert space and a complete set of Dirac observables available, we can introduce semi-classical (coherent) states and study their evolution. We first fix the time at \( \phi = \phi_o \) to construct the semi-classical state which is peaked at \( p_\phi = p_\phi^* \) and \( \vec{\mu} |_{\phi_o} = \vec{\mu}_\phi^* \).

To have a semi-classical state corresponding to a universe with the characteristic quantities much larger than Planck scales, we demand that \( \mu_\phi^* \gg \mu_I \) and \( p_\phi^* \gg \hbar \sqrt{G} \) (or equivalently \( K \kappa_\phi \gg 1 \)). At the initial time \( \phi = \phi_o \), consider the coherent state:

\[
\Psi_{\vec{\mu}_\phi^*,\vec{p}_\phi^*}(\vec{\mu},\phi_o) = \int \frac{d^3 k}{\omega^2(\vec{k})>0} \tilde{\Psi}_R(\vec{k}) e^{i \omega(\vec{k})(\phi - \phi_o^*)}, \quad (6.17)
\]

where the Fourier amplitude \( \tilde{\Psi}_R(\vec{k}) \) is given by

\[
\tilde{\Psi}_R(\vec{k}) = \frac{1}{(2\pi)^{3/4}} \frac{1}{\sqrt{\sigma_1 \sigma_2 \sigma_3}} e^{\frac{(k_1 - K\kappa_1)^2}{(2\sigma_1)^2}} e^{\frac{(k_2 - K\kappa_2)^2}{(2\sigma_2)^2}} e^{\frac{(k_3 - K\kappa_3)^2}{(2\sigma_3)^2}}, \quad (6.18)
\]

With the Dirac operators as well as the physical inner product in hand, we are able to calculate the expectation and uncertainty of the physical observables for a given physical state and thereby to extract the physics in WDW theory.

The same representation of the algebra of Dirac observables can be obtained by the more systematic group averaging method \([30, 31, 32, 33, 34]\), as has been done for the isotropic model in \([1]\). There may be some complications in anisotropic cases and we defer this issue to future study.
which is sharply (if \( \sigma_i \ll K_\kappa_i \)) peaked at \( \vec{k} = K\vec{n} \). The constants \( \mu_{\phi_0}^* \) and \( \phi_0^* \) are related by

\[
\mu_{\phi_0}^* = e^{i(2\pi)^2} e^{\sqrt{8\pi\hbar}(\frac{\kappa_2 + \kappa_3}{\sigma_0})(\phi_0^* - \phi_0)}, \\
\mu_{\phi_0}^* = e^{i(2\pi)^2} e^{\sqrt{8\pi\hbar}(\frac{1 - \kappa_1}{\kappa_0})(\phi_0^* - \phi_0)}, \\
\mu_{\phi_0}^* = e^{i(2\pi)^2} e^{\sqrt{8\pi\hbar}(\frac{\kappa_1 + \kappa_2}{\sigma_0})(\phi_0^* - \phi_0)},
\]

which are suggestive of the classical solution (3.23). Similarly, referring to (2.8), we set

\[
p_\phi^* = \hbar \sqrt{8\pi G K_{\phi_0}}.
\]

The parameters \( \kappa_{1,2,3} \) and \( \kappa_\phi \) satisfy the constraint (2.7).

As the action of the Dirac observables on the initial states and the physical inner product are well defined in (6.14) and (6.15), in Appendix A, we are able to calculate the expectations and dispersions of the Dirac observables. The results are:

- The expectation value of \( \mu_I|\phi_0 \):

\[
\langle \mu_I|\phi_0 \rangle := \langle \Psi_{\vec{\mu}_{\phi_0},p_\phi}^* | \mu_I | \phi_0 \rangle \approx \mu_{\phi_0}^*.
\]

- The dispersion square of \( \mu_I|\phi_0 \):

\[
\Delta^2(\mu_I|\phi_0) \equiv \langle (\mu_I|\phi_0)^2 \rangle - \langle \mu_I|\phi_0 \rangle^2 := \langle \Psi_{\vec{\mu}_{\phi_0},p_\phi}^* | \mu_I | \phi_0 \rangle^2 \langle \Psi_{\vec{\mu}_{\phi_0},p_\phi}^* | \mu_I | \phi_0 \rangle \approx (e^{2\pi I} - 1)(\mu_{\phi_0}^*)^2.
\]

- The expectation value of \( p_\phi \):

\[
\langle p_\phi \rangle := \langle \Psi_{\vec{\mu}_{\phi_0},p_\phi}^* | \vec{p}_{\phi} | \Psi_{\vec{\mu}_{\phi_0},p_\phi}^* \rangle \approx p_{\phi}^*.
\]

- The dispersion square of \( p_\phi \):

\[
\Delta^2(p_\phi) \equiv \langle p_\phi^2 \rangle - \langle p_\phi \rangle^2 := \langle \Psi_{\vec{\mu}_{\phi_0},p_\phi}^* | \vec{p}_{\phi}^2 | \Psi_{\vec{\mu}_{\phi_0},p_\phi}^* \rangle \approx \frac{2p_{\phi}^2}{\kappa_0^2} (\sigma_1^2(\kappa_2 + \kappa_3)^2 + \sigma_2^2(\kappa_1 + \kappa_3)^2 + \sigma_3^2(\kappa_1 + \kappa_2)^2).
\]

As the evolution of the coherent state is concerned, because of (6.11), the solution \( \Psi_{\vec{\mu}_{\phi_1},p_\phi}^*(\vec{\mu}, \phi) \) defined by the initial state \( \Psi_{\vec{\mu}_{\phi_0},p_\phi}^*(\vec{\mu}, \phi_0) \) can be obtained simply by replacing \( \phi_0 \) with \( \phi \) in (6.17). This implies that when the state is evolved to the instant \( \phi \), it is again a semi-classical state peaked at

\[
\langle \mu_I|\phi \rangle \approx e^{i(2\pi)^2} e^{\sqrt{8\pi\hbar}(\frac{1 - \kappa_1}{\kappa_0})(\phi_0^* - \phi)} \equiv \mu_{\phi_0}^*.
\]

and with the uncertainty spread:

\[
\Delta^2(\mu_I|\phi) \approx (e^{2\pi I} - 1)(\mu_{\phi_0}^*)^2.
\]
Comparing (6.19) and (6.25), we have

\[
\mu^* \phi = \mu^* \phi_o \sqrt{8\pi G \frac{1-\kappa}{\kappa}} (\phi - \phi_o),
\]

which shows that the semi-classical state continues to be peaked at the trajectory exactly described by a classical solution as in (3.23). On the other hand, \( \langle p \phi \rangle \) and \( \Delta^2(p \phi) \) are independent of time.

The fact that the semi-classical states follow the classical trajectories implies that they are destined for the singularity (Kasner-like or not) in the backward evolution. In this sense, WDW evolution does not resolve the classical singularity.

Remark: To get the semi-classical (coherent) state in the context of LQC, we simply replace \( e^{(s)}_k(\vec{\mu}) \) in (6.17) with \( e^{(s)}(\vec{\mu}) \) (the symmetrized eigenfunctions of \( \Theta \), to be defined in Section VII B). Since \( e^{(s)}(\vec{\mu}) \rightarrow e^{(s)}_k(\vec{\mu}) \) for \( |\mu| \gg \mu_o \), the wavefunction given by (6.17) is used as the initial state at late times to conduct the numerical analysis for LQC [11]. See Section VII D for more details of LQC semi-classical states.

VII. ANALYTICAL ISSUES IN LQC (\( \gamma \mu \)-SCHEME)

In this section, we come back to the model in LQC and more detailed analytical issues are explored. We include the matter sector to the Hamiltonian and show that the scalar field \( \phi \) can again be used as emergent time. The total Hamiltonian constraint gives a difference revolution equation and the general solutions to it are closely examined. The results enable us to construct the physical Hilbert and the Dirac observables. In Section VII C we also prove that the state in the kinematical Hilbert space associated with the classical singularity is completely decoupled from the evolution, which adds evidence to the occurrence of the big bounce.

A. The Total Hamiltonian Constraint (Matter Sector Included)

Since \( C_\phi = 8\pi G p_\phi^2/\sqrt{|p_1| p_2 p_3} \) in (3.22), the corresponding operator \( \hat{C}_\phi \) in LQC acting on the states of \( H_{kin}^{total} := H_{grav}^S \otimes H_\phi \) is given by

\[
\hat{C}_\phi |\vec{\mu}\rangle \otimes |\phi\rangle = \left[ \frac{1}{\sqrt{|p_1|}} \right] \left[ \frac{1}{\sqrt{|p_2|}} \right] \left[ \frac{1}{\sqrt{|p_3|}} \right] |\vec{\mu}\rangle \otimes 8\pi G \hat{p}_\phi^2 |\phi\rangle.
\]

(7.1)

According to (4.16), this gives

\[
\hat{C}_\phi^{(\gamma \mu)} |\vec{\mu}\rangle \otimes |\phi\rangle = \frac{1}{(4\pi \gamma)^{\frac{3}{2}} \ell^3_{Pl}} B(\vec{\mu}) |\vec{\mu}\rangle \otimes 8\pi G \hat{p}_\phi^2 |\phi\rangle,
\]

(7.2)

where

\[
B(\vec{\mu}) := \frac{1}{\gamma_1 \gamma_2 \gamma_3} \left| |\mu_1 + \gamma_1|^{\frac{1}{2}} - |\mu_1 - \gamma_1|^{\frac{1}{2}} \right| \times \left| |\mu_2 + \gamma_2|^{\frac{1}{2}} - |\mu_2 - \gamma_2|^{\frac{1}{2}} \right| \left| |\mu_3 + \gamma_3|^{\frac{1}{2}} - |\mu_3 - \gamma_3|^{\frac{1}{2}} \right|.
\]

(7.3)
The total Hamiltonian constraint $\hat{C}^{(n)}_{\text{grav}} + \hat{C}^{(\mu)}_{\phi} = 0$ then yields

$$8\pi G B(\vec{\mu}) \hat{p}_\phi^2 |\vec{\mu}, \phi\rangle + (4\pi)^2 \hat{C}^{(n)}_{\text{grav}} |\vec{\mu}, \phi\rangle = 0. \quad (7.4)$$

Both the classical and the WDW theories suggest that $\phi$ can be used as emergent time; i.e., $\phi$ is to be thought of as “time” while $\vec{\mu}$ as the genuine, physical degrees of freedom which evolve with respect to $\phi$. To implement the total kinematical Hilbert space with this idea, we choose the standard Schrödinger representation for $\phi$ but the “polymer representation” for $\vec{\mu}$, which captures the quantum geometry effects; that is $H^{\text{total}}_{\text{kin}} = L^2(\mathbb{R}^3_{\text{Bohr}}, d^3\mu_{\text{Bohr}}) \otimes L^2(\mathbb{R}, d\phi)$. In this representation, $\hat{p}_\phi = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$ and the total Hamiltonian constraint reads as

$$\frac{\partial^2}{\partial \phi^2} \Psi(\vec{\mu}, \phi) = \frac{\pi G}{2 \gamma_1 \gamma_2 \gamma_3} [B(\vec{\mu})]^{-1} \left\{ C_3^{++}(\vec{\mu}) \Psi(\mu_1 + 2\mu_2, \mu_2 + 2\mu_2, \mu_3, \phi) - C_3^{-+}(\vec{\mu}) \Psi(\mu_1 - 2\mu_2, \mu_2 + 2\mu_2, \mu_3, \phi) - C_3^{+-}(\vec{\mu}) \Psi(\mu_1 + 2\mu_2, \mu_2 - 2\mu_2, \mu_3, \phi) + C_3^{--}(\vec{\mu}) \Psi(\mu_1 - 2\mu_2, \mu_2 - 2\mu_2, \mu_3, \phi) \right\} \Psi(\vec{\mu}, \phi)$$

$$=: - \Theta(\mu_1, \mu_2) + \Theta_2(\mu_1, \mu_3) + \Theta_1(\mu_2, \mu_3) \Psi(\vec{\mu}, \phi)$$

$$=: - \Theta(\vec{\mu}) \Psi(\vec{\mu}, \phi), \quad (7.5)$$

where

$$C_3^{++}(\vec{\mu}) := \left| \sqrt{(\mu_1 + 2\gamma_1)\mu_2(\mu_3 + \gamma_3)} - \sqrt{(\mu_1 + 2\gamma_1)\mu_2(\mu_3 - \gamma_3)} \right|$$

$$+ \left| \sqrt{\mu_1(\mu_2 + 2\gamma_2)(\mu_3 + \gamma_3)} - \sqrt{\mu_1(\mu_2 + 2\gamma_2)(\mu_3 - \gamma_3)} \right|,$$

$$C_3^{-+}(\vec{\mu}) := \left| \sqrt{(\mu_1 - 2\gamma_1)\mu_2(\mu_3 + \gamma_3)} - \sqrt{(\mu_1 - 2\gamma_1)\mu_2(\mu_3 - \gamma_3)} \right|$$

$$+ \left| \sqrt{\mu_1(\mu_2 - 2\gamma_2)(\mu_3 + \gamma_3)} - \sqrt{\mu_1(\mu_2 - 2\gamma_2)(\mu_3 - \gamma_3)} \right|,$$

$$C_3^{+-}(\vec{\mu}) := \left| \sqrt{(\mu_1 + 2\gamma_1)\mu_2(\mu_3 - \gamma_3)} - \sqrt{(\mu_1 + 2\gamma_1)\mu_2(\mu_3 + \gamma_3)} \right|$$

$$+ \left| \sqrt{\mu_1(\mu_2 - 2\gamma_2)(\mu_3 - \gamma_3)} - \sqrt{\mu_1(\mu_2 - 2\gamma_2)(\mu_3 + \gamma_3)} \right|,$$

and similar for $C_2^{\pm\pm}$ and $C_1^{\pm\pm}$ in the cyclic manner. The coefficients $C_l^{\pm\pm}$ have the following properties:

$$C_3^{++}(0, \mu_2, \mu_3) = C_3^{-+}(0, \mu_2, \mu_3) = C_3^{+-}(0, \mu_2, \mu_3) = C_3^{--}(0, \mu_2, \mu_3),$$

$$C_3^{++}(\mu_1, 0, \mu_3) = C_3^{-+}(\mu_1, 0, \mu_3) = C_3^{+-}(\mu_1, 0, \mu_3) = C_3^{--}(\mu_1, 0, \mu_3), \quad (7.7)$$

and

$$C_3^{++}(0, 0, \mu_3) = C_3^{-+}(0, 0, \mu_3) = C_3^{+-}(0, 0, \mu_3) = C_3^{--}(0, 0, \mu_3) = 0,$$

$$C_3^{++}(\mu_1, \mu_2, 0) = C_3^{-+}(\mu_1, \mu_2, 0) = C_3^{+-}(\mu_1, \mu_2, 0) = C_3^{--}(\mu_1, \mu_2, 0) = 0, \quad (7.8)$$
for $\forall \mu_1, \mu_2, \mu_3$. ($C_{1,2}^\pm$ have the similar properties in the cyclic manner.) For later convenience, we also define

$$\tilde{C}_I^{\pm\pm}(\mu_J, \mu_K) := \frac{\pi G}{2\gamma_1\gamma_2\gamma_3}[B(\vec{\mu})]^{-1}C_I^{\pm\pm}(\vec{\mu}),$$

(7.9)

which is independent of $\mu_I$ and has the properties:

$$\tilde{C}_3^{++}(-2\gamma_1, -2\gamma_2) = \tilde{C}_3^{+-}(-2\gamma_1, 2\gamma_2) = \tilde{C}_3^{-+}(2\gamma_1, -2\gamma_2) = \tilde{C}_3^{--}(2\gamma_1, 2\gamma_2) = 0,$$

(7.10)

and

$$\tilde{C}_3^{\pm\pm}(0, \mu_2), \tilde{C}_3^{\pm\pm}(\mu_1, 0) \to \infty,$$

(7.11)

for $\forall \mu_1, \mu_2$. ($\tilde{C}_{1,2}^{\pm\pm}$ have the similar properties in the cyclic manner.) Also note that $\Theta_I$ is independent of $\mu_I$. It is easy to see that $\Theta$ and each of $\Theta_I$ individually are self-adjoint on $L^2(\mathbb{R}^3_{\text{Bohr}}, B(\vec{\mu}) d^3\mu_{\text{Bohr}})$.

**B. Emergent Time and the General Solutions**

The resulting Hamiltonian equation (7.5) is cast in the way very similar to that of the WDW constraint (6.3). The key difference is that the $\phi$-independent operator $\Theta$ is now a difference operator rather than a differential operator. In the same spirit as for WDW constraint, the LQC quantum Hamiltonian constraint can be regarded as an “evolution equation” which evolves the quantum state in the emergent time $\phi$.

As in the isotropic model, since $\Theta$ is a difference operator, the space of physical states (i.e. appropriate solutions to the constraint equation) is naturally divided into sectors, each of which is preserved by the “evolution” and by the action of the Dirac observables. Thus, there is super-selection among these sectors. Let $L_{\epsilon/f} (|\epsilon_f| \leq \gamma_1)$ be the “lattice” of points $\{|\epsilon_f| + 2n\gamma_1; n \in \mathbb{Z}\}$ on the $\mu_1$-axis, $L_{|\epsilon_f|}$ be the “lattice” of points $\{-|\epsilon_f| + 2n\gamma_1; n \in \mathbb{Z}\}$ and $L_{\epsilon_f} = L_{|\epsilon_f|} \cup L_{-|\epsilon_f|}$. Also let $\mathcal{H}^{\text{grav}}_{\pm|\epsilon_1|, \pm|\epsilon_2|, \pm|\epsilon_3|}$ (8 of them) and $\mathcal{H}^{\text{grav}}_{\epsilon}$ denote the physical subspaces of $L^2(\mathbb{R}^3_{\text{Bohr}}, B(\vec{\mu}) d^3\mu_{\text{Bohr}})$ with states whose support is restricted to the lattices $L_{\pm|\epsilon_1|} \otimes L_{\pm|\epsilon_2|} \otimes L_{\pm|\epsilon_3|}$ and $L_{\epsilon_1} \otimes L_{\epsilon_2} \otimes L_{\epsilon_3}$ respectively. Each of these subspaces is mapped to itself by $\Theta$. Furthermore, since $\tilde{C}_3^{(\epsilon)}(\vec{\mu})$ is self-adjoint on $\mathcal{H}^{\text{grav}}_{\text{kin}} = L^2(\mathbb{R}^3_{\text{Bohr}}, d^3\mu_{\text{Bohr}})$, it follows that $\Theta$ is self-adjoint on all these physical Hilbert subspaces.

Note however that since $L_{|\epsilon_f|}$ and $L_{-|\epsilon_f|}$ are mapped to each other by the operators $\Pi_I$, none of $\mathcal{H}^{\text{grav}}_{\pm|\epsilon_1|, \pm|\epsilon_2|, \pm|\epsilon_3|}$ but only $\mathcal{H}^{\text{grav}}_{\epsilon}$ is left invariant by $\Pi_{1,2,3}$. The operators $\Pi_I$ reverse the triad orientation and thus represent a large gauge transformation. In gauge theories, we have to restrict ourselves to the sector corresponding to an eigenspace of the group of large gauge transformations. Since there are no fermions and no parity violating processes in our theory, we are led to choose the symmetric sector (i.e. the subspace of $\mathcal{H}^{\text{grav}}_{\epsilon}$ in which $\Psi(\vec{\mu}) = \Psi(-\mu_1, \mu_2, \mu_3) = \Psi(\mu_1, -\mu_2, \mu_3) = \Psi(\mu_1, \mu_2, -\mu_3)$), which will be of our primary interest.

To explore the properties of the operator $\Theta$, Let us first consider a generic $\epsilon$ (i.e. none of $\epsilon_f$ equals 0 or $\gamma_1$). On each of the 8 Hilbert space $\mathcal{H}^{\text{grav}}_{\pm|\epsilon_1|, \pm|\epsilon_2|, \pm|\epsilon_3|}$, we can solve for the eigenvalue equation $\Theta e_{\lambda}(\vec{\mu}) = (\Theta_1 + \Theta_2 + \Theta_3) e_{\lambda}(\vec{\mu}) = \lambda e_{\lambda}(\vec{\mu})$. Since $\Theta_I$ is independent of
\[ \mu_1, \text{ we solve the eigenvalue problem by separating the variables; that is, let } e_\lambda(\mu_1, \mu_2, \mu_3) = e_{\lambda_1}(\mu_1) e_{\lambda_2}(\mu_2) e_{\lambda_3}(\mu_3) \text{ and solve} \]

\[
\begin{align*}
\Theta_3 e_{\lambda_{12}}(\mu_1, \mu_2) &= \lambda_{12} e_{\lambda_{12}}(\mu_1, \mu_2), \quad \text{for } e_{\lambda_{12}}(\mu_1, \mu_2) = e_{\lambda_1}(\mu_1) e_{\lambda_2}(\mu_2), \\
\Theta_2 e_{\lambda_{13}}(\mu_1, \mu_3) &= \lambda_{13} e_{\lambda_{13}}(\mu_1, \mu_3), \quad \text{for } e_{\lambda_{13}}(\mu_1, \mu_3) = e_{\lambda_1}(\mu_1) e_{\lambda_3}(\mu_3), \\
\Theta_1 e_{\lambda_{23}}(\mu_2, \mu_3) &= \lambda_{23} e_{\lambda_{23}}(\mu_2, \mu_3), \quad \text{for } e_{\lambda_{23}}(\mu_2, \mu_3) = e_{\lambda_2}(\mu_2) e_{\lambda_3}(\mu_3),
\end{align*}
\]

with \( \lambda = \lambda_{12} + \lambda_{13} + \lambda_{23} \). Each of (7.13) can be solved recursively for any arbitrary \( \lambda_{ij} \) provided that the appropriate boundary condition is given. For example, the detail of \( \Theta_3 e_{\lambda_{12}}(\mu_1, \mu_2) = \lambda_{12} e_{\lambda_{12}}(\mu_1, \mu_2) \) reads as

\[
\begin{align*}
\tilde{C}_3^{++}(\mu_1, \mu_2) e_{\lambda_{12}}(\mu_1 + 2\mu_1, \mu_2 + 2\mu_2) - \tilde{C}_3^{--}(\mu_1, \mu_2) e_{\lambda_{12}}(\mu_1 - 2\mu_1, \mu_2 - 2\mu_2) \\
- \tilde{C}_3^{-+}(\mu_1, \mu_2) e_{\lambda_{12}}(\mu_1 + 2\mu_1, \mu_2 - 2\mu_2) + \tilde{C}_3^{+-}(\mu_1, \mu_2) e_{\lambda_{12}}(\mu_1 - 2\mu_1, \mu_2 + 2\mu_2) \\
= -\lambda_{12} e_{\lambda_{12}}(\mu_1, \mu_2),
\end{align*}
\]

and since the coefficients \( \tilde{C}_3^{\pm\pm} \) never vanish or go to infinity on the generic lattice (see (7.12)), \( e_{\lambda_{12}}(\mu_1 - 2\mu_1, \mu_2 - 2\mu_2) \) can be obtained for any \( \lambda_{12} \) when the values of \( e_{\lambda_{12}}(\mu_1 + 2\mu_1, \mu_2 + 2\mu_2) \), \( e_{\lambda_{12}}(\mu_1 - 2\mu_1, \mu_2 + 2\mu_2) \), \( e_{\lambda_{12}}(\mu_1 + 2\mu_1, \mu_2 - 2\mu_2) \), \( e_{\lambda_{12}}(\mu_1 - 2\mu_1, \mu_2 - 2\mu_2) \) and \( e_{\lambda_{12}}(\mu_1, \mu_2) \) are given. (See Figure 1a.) Therefore, if the values of \( e_{\lambda_{12}}(\mu_1, \mu_2) \) are specified on the boundary lines \( \mu_1 = \mu_1^*, \mu_2 = \mu_2^* \) and \( \mu_2 = \mu_2^* - 2\mu_1 \) in the lattice \( L_{\pm\pm} \), \( e_{\lambda_{12}}(\mu_1, \mu_2) \) can be uniquely determined via the recursion relation (7.14) for all the lattice points with \( \mu_1 < \mu_1^* \) and \( \mu_2 < \mu_2^* \). (See Figure 1b.)

On the other hand, the LQC operator \( \Theta_I \) reduces to the WDW operator \( \Theta_I \) in the “asymptotic” regime (i.e. \( |\mu_I| \gg \gamma_I \)), and thus the LQC eigenfunction \( e_\lambda(\vec{\mu}) \) approaches the WDW eigenfunction \( e_\lambda(I) \) given by (6.4) for large \( |\mu_I| \). Therefore, we can use the same labels \( k_i \) to denote the LQC eigenfunctions (namely, \( \lambda_{1,2,3} = k_{1,2,3} \)) and similarly decompose

\begin{align*}
(a) & \\
(b) &
\end{align*}
\[ e_{\ell}(\vec{\mu}) \] as \( e_{k_{1}}(\mu_{1}) e_{k_{2}}(\mu_{2}) e_{k_{3}}(\mu_{3}) \). It follows that \( e_{k_{1}}(\mu_{1}) \to e_{k_{1}}(\mu_{1}) \) for \( |\mu_{1}| \gg q_{1} \) and we have the identifications:

\[ \lambda_{12} = 16\pi G \left( k_{1}k_{2} + \frac{1}{16} \right), \quad \lambda_{13} = 16\pi G \left( k_{1}k_{3} + \frac{1}{16} \right), \quad \lambda_{23} = 16\pi G \left( k_{2}k_{3} + \frac{1}{16} \right), \quad (7.15) \]

and

\[ \lambda = \omega^{2}(\vec{k}) = 16\pi G \left( k_{1}k_{2} + k_{1}k_{3} + k_{2}k_{3} + \frac{3}{16} \right). \quad (7.16) \]

Like \( \Theta \) in the WDW theory, the LQC operator \( \Theta \) is not positive definite. For the same argument we used in Section [VI.A] only those modes with \( \omega^{2} > 0 \) are allowed and what matters is just the operator \( \Theta_{+} \), obtained by projecting the action of \( \Theta \) to the positive eigenspace in its spectral decomposition.

For a given \( \vec{k} \), we can find \( e_{\lambda_{ij}} \) as mentioned above by appropriately specifying the boundaries in such a way that \( e_{\lambda_{ij}}(\mu_{1}, \mu_{j}) \to e_{k_{1}}(\mu_{1}) e_{k_{j}}(\mu_{j}) \) for \( |\mu_{1}| \gg q_{1}, |\mu_{j}| \gg q_{j} \). However, \( (6.14) \) gives \( e_{k_{1}}(\mu_{1}) e_{k_{2}}(\mu_{2}) \) = \( (4\pi)^{-2} \mu_{1}^{-1/4+i\lambda k_{1}} \mu_{2}^{-1/4+i\lambda k_{2}} \), which is not suitable to be used for the boundary condition, since one of \( \mu_{1} \) and \( \mu_{2} \) could be small on the boundary lines \( \mu_{1} = \mu_{1}^{*}, \mu_{1} = \mu_{1}^{*} - 2q_{1}, \mu_{2} = \mu_{2}^{*}, \mu_{2} = \mu_{2}^{*} - 2q_{2} \) and thus the WDW limit is not always valid even if both \( \mu_{1}^{*} \) and \( \mu_{2}^{*} \) are very big. To reflect the effect of quantum geometry for small \( \mu_{1} \) or \( \mu_{2} \), we follow the same strategy à la Thiemann’s trick used for the inverse triad operators in Section [IV.C] and designate the “tamed” function

\[ \frac{1}{(4\pi)^{2}} \left( \frac{1}{q_{1}} |\mu_{1} + q_{1} |^{\frac{1}{4}} - |\mu_{1} - q_{1} |^{\frac{1}{4}} \right)^{\frac{3}{2} - 2i\lambda k_{1}} \times \left( \frac{1}{q_{2}} |\mu_{2} + q_{2} |^{\frac{1}{4}} - |\mu_{2} - q_{2} |^{\frac{1}{4}} \right)^{\frac{3}{2} - 2i\lambda k_{2}} \quad (7.17) \]

as the value of \( e_{\lambda_{12}}(\mu_{1}, \mu_{2}) \) on the boundary, which again reduces to \( e_{k_{1}}(\mu_{1}) e_{k_{2}}(\mu_{2}) \) when both \( |\mu_{1}| \gg q_{1} \) and \( |\mu_{2}| \gg q_{2} \). In practice, we use \( (7.17) \) to specify the boundary condition on the lines \( (\mu_{1} = \mu_{1}^{*}, -\mu_{1}^{*} \leq \mu_{2} \leq \mu_{2}^{*}, \mu_{1} = \mu_{1}^{*} - 2q_{1}, -\mu_{1}^{*} \leq \mu_{2} \leq \mu_{2}^{*}, \mu_{1} = \mu_{1}^{*}, -\mu_{1}^{*} \leq \mu_{2} \leq \mu_{2}^{*} - 2q_{2}, -\mu_{1}^{*} \leq \mu_{2} \leq \mu_{2}^{*}) \) of the lattice for \( \mu_{1} \gg q_{1} \) and \( \mu_{2} \gg q_{2}, \) then the recursion relation \( (7.14) \) uniquely gives the values \( e_{\lambda_{12}}(\mu_{1}, \mu_{2}) \) for all the lattice points within the range: \(-\mu_{1}^{*} \leq \mu_{1} \leq \mu_{1}^{*} \) and \(-\mu_{2}^{*} \leq \mu_{2} \leq \mu_{2}^{*} \). The eigenfunctions so obtained are denoted as \( e_{\lambda_{12}}^{+}, e_{\lambda_{12}}^{\pm}, \ldots \) for the lattices \( \mathcal{L}_{[r]} \otimes \mathcal{L}_{[c]}, \mathcal{L}_{[r]} \otimes \mathcal{L}_{[c]} \otimes \mathcal{L}_{[c]} \ldots \) respectively. We are only interested in the symmetric sector and have to symmetrize the eigenfunctions to get:

\[ e_{\lambda_{12}}^{(s)}(\mu_{1}, \mu_{2}) = \frac{1}{\sqrt{16}} \left( e_{\lambda_{12}}^{+,+}(\mu_{1}, \mu_{2}) + e_{\lambda_{12}}^{-+,+}(\mu_{1}, -\mu_{2}) + e_{\lambda_{12}}^{-+,+}(\mu_{1}, \mu_{2}) + e_{\lambda_{12}}^{+,-,+}(\mu_{1}, -\mu_{2}) \right. \]

\[ + \cdots \]

\[ + e_{\lambda_{12}}^{+,+}(\mu_{1}, \mu_{2}) + e_{\lambda_{12}}^{-,+}(\mu_{1}, -\mu_{2}) + e_{\lambda_{12}}^{-,+}(\mu_{1}, \mu_{2}) + e_{\lambda_{12}}^{+,+}(\mu_{1}, -\mu_{2}) \right). \quad (7.18) \]

The same procedure is applied for \( e_{\lambda_{12}}^{(s)}(\mu_{1}, \mu_{3}) \) and \( e_{\lambda_{23}}^{(s)}(\mu_{2}, \mu_{3}) \). Finally, the LQC eigenfunction \( e_{\lambda_{ij}}^{(s)}(\vec{\mu}) \) in the symmetric sector can be determined for a given \( \vec{k} \) by obtaining \( e_{\lambda_{12}}, e_{\lambda_{12}} \) and \( e_{\lambda_{12}} \) separately.

The eigenfunctions in the symmetric sector of \( \mathcal{H}_{\text{grav}}^{e} \) can be normalized such that we have the orthonormality relation:

\[ \sum_{\vec{\mu} \in \mathcal{L}_{e_{1}} \otimes \mathcal{L}_{e_{2}} \otimes \mathcal{L}_{e_{3}}} B(\vec{\mu}) e_{\kappa_{1}}^{(s)}(\vec{\mu}) e_{\kappa_{2}}^{(s)}(\vec{\mu}) = \delta^{3}(\vec{k}, \vec{k}'), \quad (7.19) \]
(where the right hand side is the standard Dirac distribution) and the completeness relation:

$$
\sum_{\bar{\mu} \in \mathcal{L}_{\epsilon_1} \otimes \mathcal{L}_{\epsilon_2} \otimes \mathcal{L}_{\epsilon_3}} B(\bar{\mu}) \tilde{e}_k^{(s)}(\bar{\mu}) \Psi(\bar{\mu}) = 0 \quad \text{for } \forall k, \quad \text{iff } \Psi(\bar{\mu}) = 0
$$

(7.20)

for any symmetric $\Psi(\bar{\mu}) \in \mathcal{H}_{\epsilon}^{grav}$. Finally, any symmetric element $\Psi(\bar{\mu})$ of $\mathcal{H}_{\epsilon}^{grav}$ can be expanded as

$$
\Psi(\bar{\mu}) = \int_{\omega^2(\bar{k}) > 0} d^3k \tilde{\Psi}(\bar{k}) \tilde{e}_k^{(s)}(\bar{\mu})
$$

(7.21)

for $\tilde{e}_k^{(s)}(\bar{\mu}) \in \mathcal{H}_{\epsilon}^{grav}$.

As in the WDW theory, the general symmetric solution to the LQC constraint (7.5) can be written as

$$
\Psi(\bar{\mu}, \phi) = \int_{\omega^2(\bar{k}) > 0} d^3k \left( \tilde{\Psi}_+(\bar{k}) \tilde{e}_k^{(s)}(\bar{\mu}) e^{i\omega \phi} + \tilde{\Psi}_-(\bar{k}) \tilde{e}_k^{(s)}(\bar{\mu}) e^{-i\omega \phi} \right)
$$

(7.22)

where $\tilde{\Psi}_\pm(\bar{k})$ are in $L^2(\mathbb{R}^3, d^3k)$. For $|\mu_I| \gg \eta I$, (7.22) reduces to the solution (6.9) to the WDW equation.

If $\tilde{\Psi}_+(-\bar{k})$ vanishes, we will say that the solution is negative/positive frequency. Thus, every solution to (7.5) admits a natural decomposition into positive- and negative-frequency parts, each of which satisfies the first order differential equation in $\phi$:

$$
\frac{\partial \Psi_\pm}{\partial \phi} = \pm i \sqrt{\Theta_+} \Psi_\pm,
$$

(7.23)

where $\sqrt{\Theta_+}$ is the square-root of the positive self-adjoint operator $\Theta_+$ defined via spectral decomposition. Therefore, the solution to (7.5) with the “initial” function $\Psi_\pm(\bar{\mu}, \phi_0) = f_\pm(\bar{\mu})$ is given by:

$$
\Psi_\pm(\bar{\mu}, \phi) = e^{\pm i \sqrt{\Theta_+}(\phi-\phi_0)} \Psi_\pm(\bar{\mu}, \phi_0).
$$

(7.24)

**Remark:** In the above discussion, we considered a generic $\epsilon$. In the special cases (i.e. $\epsilon_I = 0$ or $\epsilon_I = \eta I$), some differences arise because the individual lattices are invariant under the reflection $\mu_I \rightarrow -\mu_I$ (i.e., the lattices $\mathcal{L}_{\epsilon_I}$ and $\mathcal{L}_{-\epsilon_I}$ coincide). For example, let consider the case when $\epsilon_1$ is generic and $\epsilon_2$ is special. We have $\mathcal{L}_{|\epsilon_2|} = \mathcal{L}_{-|\epsilon_2|} = \mathcal{L}_{\epsilon_2}$ and $e^{++} = e^{+-}$. Consequently, the symmetrization of (7.18) should be modified to

$$
e^{(s)}_{\lambda_12}(\mu_1, \mu_2) = \frac{1}{\sqrt{8}} \left( e^{++}_{\lambda_12}(\mu_1, \mu_2) + e^{++}_{\lambda_12}(\mu_1, -\mu_2) + e^{++}_{\lambda_12}(-\mu_1, \mu_2) + e^{++}_{\lambda_12}(-\mu_1, -\mu_2) \\
+ e^{-+}_{\lambda_12}(\mu_1, \mu_2) + e^{-+}_{\lambda_12}(\mu_1, -\mu_2) + e^{-+}_{\lambda_12}(-\mu_1, \mu_2) + e^{-+}_{\lambda_12}(-\mu_1, -\mu_2) \right).
$$

(7.25)

Furthermore, if both $\epsilon_1$ and $\epsilon_2$ are special, we have $e^{++} = e^{++} = e^{-+} = e^{-+}$ and the symmetrization is performed as

$$
e^{(s)}_{\lambda_12}(\mu_1, \mu_2) = \frac{1}{\sqrt{4}} \left( e^{++}_{\lambda_12}(\mu_1, \mu_2) + e^{++}_{\lambda_12}(\mu_1, -\mu_2) + e^{++}_{\lambda_12}(-\mu_1, \mu_2) + e^{++}_{\lambda_12}(-\mu_1, -\mu_2) \right).
$$

(7.26)

In the numerical computation, we can focus on the lattice of the special case with $\epsilon = \tilde{\omega}_2$ and take advantage of the fact that $\mathcal{L}_{+|\epsilon_I|} = \mathcal{L}_{-|\epsilon_I|}$. Therefore, we restrict ourselves to the positive $\mu_{1,2,3}$
and the tedious procedure of symmetrization can be avoided. This way, the numerical computation is much more efficient.

There is a further subtlety when the recursion relation (7.11) is applied to the lattice $L_{e_1} \otimes L_{e_2}$ with $e_1 = 0$ or $e_2 = 0$, because the coefficients $\tilde{C}_3^{\pm \pm}$ may vanish or go to infinity at some lattice points and thus more careful consideration is needed. This issue is closely related to the resolution of the singularity and the detail of it is studied in Section VIIIC.

C. Resolution of the Singularity and Comments on the Planar Collapse

What is the fate of the classical singularity and planar collapse? In the classical dynamics, the Kasner-like solutions (two of $\kappa_i$ positive, the other negative) approach the Kasner-like singularity as $\phi \to -\infty$ and the planar collapse as $\phi \to -\infty$ (with $\kappa_{\phi} > 0$), whereas the Kasner-unlike solutions ($0 < \kappa_1, \kappa_2, \kappa_3 < 1$) encounter the Kasner-unlike singularity as $\phi \to -\infty$ and no planar collapse. Since $1 - \kappa_i > 0$, according to (3.23), the singularity (both Kasner-like and Kasner-unlike) gives $p_1, p_2, p_3 \to 0$, which corresponds to the state $|0, 0, 0\rangle$ on $H^{grav}_S$ and thus the point $(0, 0)$ on the lattice $L_{e_1} \otimes L_{e_2}$. On the other hand, by (3.23) again, the planar collapse gives $(p_1, p_2, p_3) \to (\infty, \infty, \infty)$, which corresponds to the state $|\infty, \infty, \infty\rangle$ on $H^{grav}_S$ and thus the point $(\infty, \infty)$ on the lattice $L_{e_1} \otimes L_{e_2}$. We first show that the state associated with the singularity is decoupled and thus the quantum evolution does not break down; later, the behaviors of the planar collapse are commented.

Unlike the classical theory, the quantum evolution does not stop at the singularity. If one begins with a generic lattice, the discrete evolution determined by (7.3) just “jumps” over the states with $\mu_f = 0$ without encountering any subtleties. The subtleties occur only on the special lattice as remarked in the end of Section VIIIB. Thus, we revisit the recursion relation (7.11) for the two special lattices: (i) $L_{e_1 = 0} \otimes L_{e_2 \neq 0}$ and (ii) $L_{e_1 = 0} \otimes L_{e_2 = 0}$.

On the special lattice $L_{e_1 = 0} \otimes L_{e_2 \neq 0}$, the boundary condition given by (7.17) implies that $e_{\lambda_{12}}(\mu_1 = 0, \mu_2 \to \infty) = 0$ and thus the state $|\mu_1 = 0, \mu_2 \to \infty\rangle$ on $H^{grav}_{e_1 = 0, \pm |e_2|}$ (marked ◦ in Figure 2) decouples from the rest part. On the other hand, the values of $e_{\lambda_{12}}(\mu_1, \mu_2)$ in the first and fourth quadrants (marked × in Figure 2a) can be obtained by direct iterating (7.14) while the recursion relation may not work for the values at $\mu_1 = -2^p \mu_1$ (points marked ◼ in Figure 2b) since the coefficients $\tilde{C}_3^{\pm \pm}(0, \mu_2)$ blow up by (7.11). However, this problem is merely artificial. To faithfully express the recursion relation, (7.14) can be rewritten as

$$C_3^{\pm \pm}(-\mu) e_{\lambda_{12}}(\mu_1 + 2^p \mu_1, \mu_2 + 2^q \mu_2) - C_3^{\pm \pm}(\mu) e_{\lambda_{12}}(\mu_1 - 2^q \mu_1, \mu_2 + 2^p \mu_2)
-C_3^{\pm \pm}(\mu) e_{\lambda_{12}}(\mu_1 + 2^q \mu_1, \mu_2 - 2^p \mu_2) + C_3^{\pm \pm}(\mu) e_{\lambda_{12}}(\mu_1 - 2^p \mu_1, \mu_2 - 2^q \mu_2)
= -B(\mu) e_{\lambda_{12}}(\mu_1, \mu_2).$$

(7.27)

Provided $B(0, \mu_2, \mu_3)\lambda_{12} = 0$ [Note: $B(0, \mu_2, \mu_3) = B(\mu_1, 0, \mu_3) = B(\mu_1, \mu_2, 0) = 0$ by its nature], the relation in (7.7) then gives

$$e_{\lambda_{12}}(2^p \mu_1, \mu_2 + 2^q \mu_2) = e_{\lambda_{12}}(2^p \mu_1, \mu_2 - 2^q \mu_2) + e_{\lambda_{12}}(2^q \mu_1, \mu_2 + 2^p \mu_2)
-e_{\lambda_{12}}(-2^q \mu_1, \mu_2 + 2^p \mu_2),$$

(7.28)

which can be used to determine the values of $e_{\lambda_{12}}$ at the points marked ◼ without difficulty. Furthermore, if the boundary condition is given symmetric under $\mu_1 \to -\mu_1$, we then have $e_{\lambda_{12}}(2^p \mu_1, \mu_2 + 2^q \mu_2) = e_{\lambda_{12}}(-2^q \mu_1, \mu_2 + 2^p \mu_2)$ and (7.28) yields $e_{\lambda_{12}}(2^p \mu_1, \mu_2 + 2^q \mu_2) = e_{\lambda_{12}}(2^q \mu_1, \mu_2 - 2^p \mu_2)$, which, as expected, tells that the values at ◼ are the exact mirrors.
evolution remains deterministic with the singularity resolved. As a result, the point (the origin) of the relation among the four points marked symmetric boundary condition, the consistency relation (7.29) is the mirror (reflected by the line \( \mu_1 = 0 \)) of the lattice \( \mathcal{L}_{s_{\mu_1}} \) and \( \mathcal{L}_{s_{\mu_2}} \). The points marked \( \circ \) are the places whose values can be easily obtained, while those with \( \odot \), \( \square \) and \( \otimes \) require more careful consideration. (The largeness of \( \mu_1^* \) and \( \mu_2^* \) is assumed but not properly presented in this figure.)

FIG. 2: (a): The lattice \( \mathcal{L}_{s_{\mu_1}} \otimes \mathcal{L}_{s_{\mu_2}} \neq 0 \). (b): The lattice \( \mathcal{L}_{s_{\mu_1}} = 0 \otimes \mathcal{L}_{s_{\mu_2}} = 0 \). The points marked \( \bullet \) are the boundary lines with given values; in particular, \( \circ \) denotes the boundary points at which the value of \( e_{\lambda_{12}} \) vanishes. The points marked \( \times \) are the places whose values can be obtained only to the first, second and fourth quadrants plus two extra points (all marked \( \otimes \)). When the recursion relation is applied for the value at the origin \( (\mu_1 = \mu_2 = 0, \text{marked } \otimes) \), the vanishing of \( \widetilde{C}_{3}^{-}(2^\lambda_{\mu_1}, 2^\lambda_{\mu_2}) \) by (7.10) makes (7.14) a consistency relation:

\[
\begin{align*}
\widetilde{C}_{3}^{++}(2^\mu_{\mu_1}, 2^\mu_{\mu_2}) e_{\lambda_{12}}(4^\mu_{\mu_1}, 4^\mu_{\mu_2}) &- \widetilde{C}_{3}^{+-}(2^\mu_{\mu_1}, 2^\mu_{\mu_2}) e_{\lambda_{12}}(0, 4^\mu_{\mu_2}) = 0 \\
-\widetilde{C}_{3}^{+-}(2^\mu_{\mu_1}, 2^\mu_{\mu_2}) e_{\lambda_{12}}(4^\mu_{\mu_1}, 0) + \lambda_{12} e_{\lambda_{12}}(2^\mu_{\mu_1}, 2^\mu_{\mu_2}) & = 0
\end{align*}
\]

and leaves the value of \( e_{\lambda_{12}}(0, 0) \) undetermined. Nevertheless, thanks to (7.10) again, the values of \( e_{\lambda_{12}} \) at the points marked \( \square \) can still be determined without knowing the value at \( \otimes \). Moreover, if the Hilbert space \( H_{s_{\mu_1}, s_{\mu_2}} \) is restricted to the symmetric sector, given the symmetric boundary condition, the consistency relation (7.29) is the mirror (reflected by the origin) of the relation among the four points marked \( \square \) and therefore it is automatically satisfied. As a result, the point \( \otimes \) is completely decoupled and the iteration “jumps” over the origin to those points marked \( \square \) and consequently to all the unmarked points in Figure 2b.

Put all together, it follows that the states associated with the point marked \( \circ \) and \( \otimes \) in Figure 2 are irrelevant. The same arguments can be easily applied for the special lattices in \( (\mu_1, \mu_3) \) - and \( (\mu_2, \mu_3) \) -planes in the cyclic manner. In the end, combining \( e_{\lambda_{12}}(\mu_1, \mu_2) \), \( e_{\lambda_{31}}(\mu_1, \mu_3) \) and \( e_{\lambda_{23}}(\mu_2, \mu_3) \) to get \( e_{\lambda_{k}}^{(s)}(\vec{p}) \), we conclude that the state \( |0, 0, 0\rangle \) associated with the singularity on \( H_{\text{grav}}^{S} \) is completely decoupled from the difference evolution and the evolution remains deterministic across the deep Planck regime. Consequently, the classical singularity (both Kasner-like and Kasner-unlike) is expected to be resolved in the quantum
evolution. (The absence of the Kasner singularity has been shown in [35] using an effective classical Hamiltonian obtained from loop quantization of vacuum Bianchi I model. Here, inclusion of the scalar field $\phi$ allows us to prove the absence of the singularity on the exact evolution equation as $\phi$ being the emergent time.)

When the matter sector is included to the model, the directional factor defined as $\varrho_I := p^2_\phi / |p_I|^3$ for any of the diagonal directions with the constant of motion $p_\phi$ plays the same role as the matter density $\rho := \frac{1}{2}p^2_\phi / |p_1 p_2 p_3|$ does in the isotropic case. The fact that the problematic state is decoupled suggests that the directional factor in any diagonal direction cannot go to infinity when the quantum discreteness is imposed. Therefore, the classical singularity (which gives infinite directional factors) is expected to be resolved and replaced by the big bounce in LQC. However, following the lesson we learned for the isotropic model in [1], the critical value of the directional factor can be arbitrarily small by increasing $p_\phi$ since we are now adopting a $\mu$-scheme. Later in Section VIII the dynamics will be refined in $\mu$-scheme, by which this problem is supposed to be fixed and the critical value for $\varrho_I$ is expected to be $O(\hbar \ell^{-4}_P)$, independent of $p_\phi$. (This has been shown for the effective dynamics in [12].)

The argument here is essentially the generalization of that used for the isotropic case in [6]. The result solidifies the assertion that the key features responsible for the resolution of the singularity are robust [21] and persist in more complicated cosmological models [5]. However, the proof presented here only shows the decoupling of the state in the kinematical Hilbert space associated with the classical singularity, but details of the dynamical behaviors of the solutions have yet to be investigated. To draw the definitive conclusion that the singularity is resolved and replaced by the bounce for those states which are semi-classical at late times, we have to figure out the physical Hilbert space, Dirac observables and semi-classical states, (which will be the topic of Section VIDA) and afterwards a thorough numerical investigation can be initiated [11].

Remark: The proof in this subsection is rather general, insensitive to the details of the matter sector. As far as the matter sector is concerned, the only proviso to make the above argument valid is: $B(0, \mu_2, \mu_3)\lambda_{12} = B(\mu_1, 0, \mu_3)\lambda_{12} = 0$, etc. By (7.15) and (7.16), this condition is equivalent to: $-B(\vec{\mu})\Theta(\vec{\mu}) = \tilde{C}_{\text{matter}}(\vec{\mu}) \to 0$, when any of $\mu_I$ goes to zero. That is, $\tilde{C}_{\text{matter}}(\vec{\mu})$ annihilates $\Psi(\vec{\mu}, \phi)$ ($\phi$ represents the matter field in general) for $\mu_1 = 0$, $\mu_2 = 0$ or $\mu_3 = 0$, which is the case for the minimally coupled matter source [4, 17].

Without the discreteness imposed for the inverse triad operator, $B(\vec{\mu})$ goes to infinity when $\mu_I \to 0$ and the above proviso no longer holds. The finiteness of the eigenvalue of $1 / \sqrt{|p_I|}$ mentioned in Section IVC therefore plays an important role for the decoupling of the singularity. However, the results of both effective dynamics and the detailed numerical analysis in isotropic models tell us: it is the “non-locality” of the gravity (i.e, $\hat{c}_I$ replaced by holonomy), not the finiteness of the inverse triad operator, that accounts for the occurrence of the big bounce and in fact the bounce takes place much earlier before the discreteness correction on the inverse triad operator becomes significant.

9 Note that, unlike the isotropic case, it is the directional factor $\varrho_I$ (not the matter density $\rho$) that indicates the happening of the big bounce. Near the epoch of the singularity, the three directional factors $\varrho_I$ may approach their critical values at slightly different instants. Therefore, the detailed occurrence of the big bounce may happen as many as three times, not just once.
Nevertheless, the fact that the problematic state is decoupled kinematically is still important, giving the lowest bound at the deep Planck regime, sometime before which the bounce should take place. For the semi-classical states at late times, however, the exact point at which the bounce occurs depends on the detailed dynamics and it is very likely to happen much earlier before the lowest bound as in the case of the isotropic model. Likewise, in the anisotropic model, we also anticipate the same situation, and accordingly expect the directional factor \( g_I \) as the indication of happening of the bounce \[12\].

Contrary to the resolution of the singularity shown above, the state \( |\infty, \infty, \infty\rangle \) on \( \mathcal{H}_{grav}^S \) associated with the planar collapse is not decoupled but persists in the evolution equation. This fact is somewhat undesirable since it means one of the length scale factors \( a_I \) continues the vanishing behavior in the forward evolution and thus eventually enters the deep Planck length scale without a stop. On the other hand, however, this is expected as the classical solutions yield \( \mu_{IC1} \to 0 \) toward the planar collapse and therefore the quantum corrections become more and more negligible. (This remains true in \( \bar{\mu} \)-scheme since \( \mu_{IC1} \to 0 \). For more details of the effectiveness of quantum corrections, see \[12\].) It can also be understood as follows. The planar collapse corresponds to the point \( (\infty, \infty, \infty) \) in the lattice \( L_{\epsilon_1} \otimes L_{\epsilon_2} \otimes L_{\epsilon_3} \), and for the points with large values of \( p_I \) the lattice discreteness can be ignored. In terms of \( p_I \), nothing is really collapsing and the classical solution toward the planar collapse is perfectly well-behaved if we treat \( p_I \) as the fundamental variables.

The result suggests that smallness of \( p_I \) (not of \( a_I \)) is the indication for the significance of quantum effect and thus also for the occurrence of bounces. While \( a_I \) are the length scale factors, \( p_I \) can be interpreted as the area scale factors according to \[3.15\]. This seems to support the speculation: “area is more fundamental than length in LQG”, although whether this is simply a technical issue or reflects some deeper facts is still unclear. (See Section VII.B of \[36\] for some comments on this aspect and \[37\] for more discussions.) Meanwhile, whereas the length operator has been shown to also have a discrete spectrum \[38\], the fact that the vanishing of the length scale factor is not resolved seems to contradict the discreteness of the length spectrum. Whether we have missed some important ingredients when imposing the discreteness corrections from the full theory or indeed area is more essential than length remains an open question for further investigation.

D. The Physical Sector and Semi-Classical States

Results of Section VII.A and Section VII.B show that while the LQC operator \( \Theta \) differs from the WDW operator \( \Theta \) in an interesting way, the structural forms of these two Hamiltonian constraint equations are quite the same. Therefore, in the LQC theory, apart from the issue of super-selection, we can introduce the Dirac observables and identify the physical Hilbert space with the inner product by demanding that the Dirac observables be self-adjoint (or by carrying out group averaging method) in the way closely analogous to what we did in WDW theory.

The super-selection sector of the physical Hilbert space \( \mathcal{H}_{\text{phys}}^{\bar{c}} \), labeled by \( \bar{c} \in [0, \bar{\gamma}_{\mu_1}] \times [0, \bar{\gamma}_{\mu_2}] \times [0, \bar{\gamma}_{\mu_3}] \) consists of the positive frequency solutions \( \Psi(\bar{\mu}, \phi) \) to (7.5) with initial data \( \Psi(\bar{\mu}, \phi_o) \) in the symmetric sector of \( \mathcal{H}_{grav}^S \). By (7.22), the explicit expression of \( \Psi(\bar{\mu}, \phi) \) in
terms of the symmetric eigenfunctions $e^{(s)}_k$ reads as

$$\Psi(\vec{\mu}, \phi) = \int \omega^2(\vec{k}) > 0 d^3k \, \tilde{\Psi}(\vec{k}) e^{(s)}_k(\vec{\mu}) e^{i\omega(\vec{k})},$$

(7.30)

where, as in the WDW theory, $\omega^2(\vec{k}) = 16\pi G(k_1k_2 + k_1k_3 + k_2k_3 + 3/16)$. The physical inner product is given by

$$\langle \Psi_1 | \Psi_2 \rangle_{\text{phy}} = \sum_{\vec{\mu} \in \mathcal{L}_1 \otimes \mathcal{L}_2 \otimes \mathcal{L}_3} B(\vec{\mu}) \tilde{\Psi}_1(\vec{\mu}, \phi_o) \Psi_2(\vec{\mu}, \phi_o).$$

(7.31)

The action of the Dirac observables is independent of $\tilde{\epsilon}$ and has the same form as in the WDW theory:

$$\hat{\mu}_I \Psi(\vec{\mu}, \phi) = e^{i\sqrt{\Theta} (\phi - \phi_o)} |\mu_I\rangle \Psi(\vec{\mu}, \phi_o) \quad \text{and} \quad \hat{p}_\phi \Psi(\vec{\mu}, \phi) = -i\hbar \frac{\partial \Psi(\vec{\mu}, \phi)}{\partial \phi}.$$  

(7.32)

The kinematical Hilbert space $\mathcal{H}_{\text{kin}}^{\text{total}}$ is non-separable but, because of super-selection, each physical sector $\mathcal{H}_{\text{phys}}^\epsilon$ is separable. The eigenvalues of the Dirac observable $\hat{\mu}_I |\phi_o\rangle$ constitute a discrete subset of the real line in each sector. In $\mathcal{H}_{\text{kin}}^{\text{grav}}$, on the contrary, the spectrum of $\hat{p}_I$ is discrete in a subtler sense: every real value is allowed but the spectrum space has discrete topology. Therefore, the more delicate discreteness of the spectrum of $\hat{p}_I$ on $\mathcal{H}_{\text{kin}}^{\text{grav}}$ descends to the standard type of discreteness of the Dirac observables on each physical sector $\mathcal{H}_{\text{phys}}^\epsilon$.

Furthermore, comparing (7.30) with the WDW semi-classical state given by (6.17), by analogy, we can construct the LQC semi-classical state at the time $\phi = \phi_o$:

$$\Psi_{\tilde{\mu}_o, \phi_o}(\vec{\mu}, \phi) = \int \omega^2(\vec{k}) > 0 d^3k \, \tilde{\Psi}(\vec{k}) e^{(s)}_k(\vec{\mu}) e^{i\omega(\vec{k})\phi_o},$$

(7.33)

where the Fourier amplitude $\tilde{\Psi}(\vec{k})$ is given by

$$\tilde{\Psi}(\vec{k}) = \tilde{\Psi}_k(\vec{k}) e^{-i\omega(\vec{k})\phi_o}$$

(7.34)

with the same $\tilde{\Psi}_k(\vec{k})$ and $\phi_o^*$ as defined in (6.18) and (6.19). Since $e^{(s)}_k(\vec{\mu}) \rightarrow e^{(s)}_\tilde{\mu}(\vec{\mu})$ for $|\mu_I| \gg \mu_I$, the wavefunction given by (7.33) is very close to that in (6.17) for large $|\mu_I|$. Therefore, the LQC semi-classical state is peaked at the classical trajectory for the region far away from the singularity and thus satisfies the pre-classicality \cite{39, 40} (at least for one asymptotic side of the evolution).

It has been argued in \cite{41} that only the zero solution satisfies the pre-classical condition for both the vacuum case and the addition of a cosmological constant in the Bianchi I model. Inclusion of matter changes the situation as suggested in \cite{41}; here, with $\phi$ being the emergent time, the LQC semi-classical states are constructed and shown to be pre-classical.

We have shown in Section VII C that the quantum evolution is deterministic, but the question whether the solution is pre-classical again on the other side across the singularity or descends into a quantum foam needs more investigation. Although the thorough numerical analysis is awaited to be done \cite{11}, the occurrence of the big bounce has been shown in \cite{12} and it turns out that the semi-classical states are pre-classical on both asymptotic sides of the evolution. (For the issues of pre-classicality and time asymmetry on either side of the evolution in the vacuum Bianchi I model, see \cite{12, 12}.)
VIII. IMPROVED DYNAMICS (µ-SCHMHE)

Section V – Section VII complete the analytical investigation for the precursor strategy (µ-scheme). In this section, we repeat the whole analysis for the improved dynamics (µ-scheme), which was first proposed and studied for the isotropic model in [8]. The prescription to endow the fundamental discreteness from the full theory is modified and implemented in a more sophisticated way, thus more directly conveying the underlying physics of quantum geometry. The corresponding WDW theory is unchanged but recast in Section VIII C featuring the use of affine variables (to be defined soon).

A. Gravitational Constraint Operator

Fixing the µ-ambiguity by setting µ to the finite number can be understood as the imprint of the fundamental discreteness of the full theory. In the full theory of LQG, a proper regularization procedure is taken to define the Hamiltonian operator: the 3d coordinate space is partitioned into small regions of coordinate volume ³. When acting on the diffeomorphism equivalence classes, the dependence on ³ is gone when ³ is smaller than some particular value because of the diffeomorphism invariance. Therefore, the Hamiltonian constraint is independent of the regulator in the end, simply because making the partition finer cannot change anything below the Planck scale [24, 25, 26].

In the symmetry reduced theory, since the diffeomorphism invariance is gauge fixed in the beginning, the independence of the regulator is no longer true and we have to fix the regulator by hand. However, the strategy used in µ-scheme is rather heuristic: the holonomy \( h^{(\mu)}(\alpha, j, I) \) in (5.8) is not a “state” of the Hilbert space and thus setting its “eigenvalue” to the area gap is not completely physical. To reflect the fundamental discreteness more rigourously, we introduce the improved strategy: “µ-scheme”.

In Cyl of the full theory, the area operator \( \hat{A}(S) \) for a coordinate surface yields quantized spectrum when acting on the spin network states |µ, j, I⟩. To carry the parallel from the full theory to the reduced theory, first, recall that the states N|µ⟩ in Cyl are analogous to the spin network states N|µ, j, I⟩ in Cyl. Second, note that the area operator \( \hat{A}(S) \) in Cyl is replaced by \( E(S_I := E(S_I, f_I = 1) \) in Cyl defined in (4.4).

Let \( S(\mu_3) \) be the square surface normal to the z-direction (with respect to µ) with the side lengths \( \mu_3 L_1 \) and \( \mu_3 L_2 \) (with respect to µ) in x- and y-directions respectively. According to (4.4), when acting on the state |µ⟩, the area operator associated with \( S(\mu_3) \) gives

\[
E(S(\mu_3))|\mu⟩ = 4\pi\gamma\ell_{pl}^2 \mu_3^2 |\mu⟩. \tag{8.1}
\]

If \( S(\mu_3) \) is the smallest area we can shrink to, we should then have \( 4\pi\gamma\ell_{pl}^2 \mu_3^2 = \pm \Delta \) or

\[
|\mu_3^2| = k := \Delta/(4\pi\gamma\ell_{pl}^2) = \sqrt{3}/2. \tag{8.2}
\]

In the other two directions, we set \( S(\mu_1) \) and \( S(\mu_2) \) to the smallest area and have the similar results: \( |\mu_1^2| = |\mu_2^2| = k \). Therefore, to faithfully reflect the area gap in the full theory, instead of the µ-scheme used earlier, we should set

\[
\bar{\mu}_1 = \frac{k}{|\mu_1|}, \quad \bar{\mu}_2 = \frac{k}{|\mu_2|}, \quad \bar{\mu}_3 = \frac{k}{|\mu_3|}. \tag{8.3}
\]
Unlike $\mu$-scheme, in which $\mu_1$ are fixed as constant, in the improved strategy, the values $\bar{\mu}_I$ to be set to fix the regulator depend adaptively on the state $|\bar{\mu}\rangle$. This is due to the presence of the operator $p_I$ in (4.4).

To figure out what the action of the operator $e^{\pm \frac{i}{\hbar} \bar{\mu}(i) c(I)}$ is when acting on $|\bar{\mu}\rangle$, we first recall that the first line of (4.17) corresponds to $e^{\mp \mu_1 \frac{\partial}{\partial \mu_1}} \psi(\mu_1, \mu_2, \mu_3) = \psi(\mu_1 \mp \mu_1, \mu_2, \mu_3)$; that is, $c^I = 2i \frac{\partial}{\partial \mu_I}$ in the $\bar{\mu}$-representation. By the same spirit, we define the affine parameter $v_I$ such that

$$\bar{\mu}(i) \frac{\partial}{\partial \mu(i)} = \sqrt{\frac{k}{|\mu_I|}} \frac{\partial}{\partial \mu_I} := \frac{\partial}{\partial v_I},$$

which leads to

$$v_I = \text{sgn}(\mu_I) \frac{2}{3 \sqrt{k}} |\mu_I|^{3/2}.$$ (8.4) (8.5)

Changing the coordinates $\mu_1, \mu_2, \mu_3$ to $v_1, v_2, v_3$, we then have

$$e^{\mp \mu_1 \frac{\partial}{\partial \mu_1}} \psi(\mu_1, \mu_2, \mu_3) = e^{\mp \frac{\partial}{\partial \mu_1}} \psi(v_1, v_2, v_3) = \psi(v_1 \mp 1, v_2, v_3),$$ (8.6)

or equivalently

$$e^{\pm \frac{i}{\hbar} \bar{\mu}(i) c(I)} |\mu_1, \mu_2, \mu_3\rangle = |v_1 \pm 1, v_2, v_3\rangle.$$ (8.7)

In terms of the new variables, that is

$$e^{\pm \frac{i}{\hbar} \bar{\mu}(i) c^I} |\bar{\nu}\rangle = |v_1 \pm 1, v_2, v_3\rangle,$$

$$e^{\pm \frac{i}{\hbar} \bar{\mu}(i) c^I} |\bar{\nu}\rangle = |v_1, v_2 \pm 1, v_3\rangle,$$

$$e^{\pm \frac{i}{\hbar} \bar{\mu}(i) c^I} |\bar{\nu}\rangle = |v_1, v_2, v_3 \pm 1\rangle.$$ (8.8)

In $\bar{\mu}$-scheme, the new operators corresponding to (5.9) and (5.10) are obtained by replacing $\mu_I$ with $\bar{\mu}_I$. Consequently, when acting on the states labeled by $v_1, v_2, v_3$, (5.11) is modified to

$$\hat{C}_{\text{grav}}^I|v_1, v_2, v_3\rangle = \frac{1}{16 \pi^2 \hbar^2 |\bar{\mu}_1| |\bar{\mu}_2| |\bar{\mu}_3|} \times \left\{ \left( \left| V_{v_1+v_2+v_3+1} - V_{v_1+v_2+v_3-1} \right| + \left| V_{v_1+v_2+v_3+1} - V_{v_1+v_2+v_3-1} \right| \right) |v_1+2, v_2+2, v_3\rangle \right. - \left( \left| V_{v_1-v_2+v_3+1} - V_{v_1-v_2+v_3-1} \right| + \left| V_{v_1-v_2+v_3+1} - V_{v_1-v_2+v_3-1} \right| \right) |v_1-2, v_2+2, v_3\rangle \\
- \left( \left| V_{v_1+v_2-v_3+1} - V_{v_1-v_2-v_3-1} \right| + \left| V_{v_1+v_2-v_3+1} - V_{v_1-v_2-v_3-1} \right| \right) |v_1+2, v_2-2, v_3\rangle + \left. \left( \left| V_{v_1-v_2-v_3+1} - V_{v_1-v_2-v_3-1} \right| + \left| V_{v_1-v_2-v_3+1} - V_{v_1-v_2-v_3-1} \right| \right) |v_1-2, v_2-2, v_3\rangle \right. + \text{cyclic terms} \right\}$$ (8.9)

\footnote{In the ordinary quantum mechanics, $p = -\frac{i}{\hbar} \frac{d}{dx}$ and $e^{ia \sigma \mu_1 / \hbar} \psi(x) = \psi(x + a)$ but we cannot simply take $e^{i f(x) \sigma p / \hbar} \psi(x) = e^{f(x) \sigma \frac{p}{\hbar}}$ because it is not unitary in general. Here, on the contrary, since CyL$_S$ is in the “polymer representation” and the right hand side of (4.7) is the Kronecker delta (not the Dirac distribution), the same problem does not occur. In fact, $\mathcal{H}_{\text{kin}}^{\text{grav}} = L^2(\mathbb{R}^3_{\text{Bohr}}, d^3 \mu_{\text{Bohr}}) = L^2(\mathbb{R}^3_{\text{Bohr}}, d^3 v_{\text{Bohr}})$ and $e^{\pm \frac{i}{\hbar} \bar{\mu}(i) c(I)}$ is unitary.}
and (5.12) is modified to

\[ \hat{\mathcal{C}}_{\text{grav}}^{(\mu)}|v_1, v_2, v_3\rangle = \frac{1}{16\pi^3 \ell_{\text{P}}^3} \cdot \frac{3\sqrt{k}}{2} \left\{ C_3^+(\vec{\nu}) \left| v_1 + 2, v_2 + 2, v_3 \right\rangle - C_3^-(\vec{\nu}) \left| v_1 - 2, v_2 + 2, v_3 \right\rangle - C_3^{++}(\vec{\nu}) \left| v_1 + 2, v_2 - 2, v_3 \right\rangle + C_3^{--}(\vec{\nu}) \left| v_1 - 2, v_2 - 2, v_3 \right\rangle \right\} + \text{cyclic terms}, \quad (8.10) \]

where the eigenvalues of the volume operator are given by

\[ V_{v_1,v_2,v_3} := (4\pi)^{3/2} \frac{3\sqrt{k}}{2} |v_1v_2v_3|^{1/3} \ell_{\text{P}}^3. \quad (8.11) \]

In terms of the new notation, it is equivalent to

\[ \hat{\mathcal{C}}_{\text{grav}}^{(\mu)}|v_1, v_2, v_3\rangle = \frac{\sqrt{2}}{2\gamma^2 \mu_1 \mu_2 \mu_3} \left\{ C_3^+(\vec{\nu}) \left| v_1 + 2, v_2 + 2, v_3 \right\rangle - C_3^-(\vec{\nu}) \left| v_1 - 2, v_2 + 2, v_3 \right\rangle - C_3^{++}(\vec{\nu}) \left| v_1 + 2, v_2 - 2, v_3 \right\rangle + C_3^{--}(\vec{\nu}) \left| v_1 - 2, v_2 - 2, v_3 \right\rangle \right\}, \quad (8.12) \]

where

\[ C_3^+(\vec{\nu}) := \frac{3\sqrt{k}}{2} \left( \left| (v_1 + 2)v_2(v_3 + 1) \right|^{1/3} - \left| (v_1 + 2)v_2(v_3 - 1) \right|^{1/3} \right) + \left| v_1(v_2 + 2)(v_3 + 1) \right|^{1/3} - \left| v_1(v_2 + 2)(v_3 - 1) \right|^{1/3} \right), \]

\[ C_3^-(\vec{\nu}) := \frac{3\sqrt{k}}{2} \left( \left| (v_1 - 2)v_2(v_3 + 1) \right|^{1/3} - \left| (v_1 - 2)v_2(v_3 - 1) \right|^{1/3} \right) + \left| v_1(v_2 - 2)(v_3 + 1) \right|^{1/3} - \left| v_1(v_2 - 2)(v_3 - 1) \right|^{1/3} \right), \]

\[ C_3^{++}(\vec{\nu}) := \frac{3\sqrt{k}}{2} \left( \left| (v_1 + 2)v_2(v_3 + 1) \right|^{1/3} - \left| (v_1 + 2)v_2(v_3 - 1) \right|^{1/3} \right) + \left| v_1(v_2 - 2)(v_3 + 1) \right|^{1/3} - \left| v_1(v_2 - 2)(v_3 - 1) \right|^{1/3} \right), \]

\[ C_3^{--}(\vec{\nu}) := \frac{3\sqrt{k}}{2} \left( \left| (v_1 - 2)v_2(v_3 + 1) \right|^{1/3} - \left| (v_1 - 2)v_2(v_3 - 1) \right|^{1/3} \right) + \left| v_1(v_2 + 2)(v_3 + 1) \right|^{1/3} - \left| v_1(v_2 + 2)(v_3 - 1) \right|^{1/3} \right) \quad (8.13) \]

and similar for \( C_2^{\pm\pm} \) and \( C_1^{\pm\pm} \) in the cyclic manner.

By inspection, it is clear that \( \hat{\mathcal{C}}_{\text{grav}}^{(\mu)'} \) and \( \hat{\mathcal{C}}_{\text{grav}}^{(\mu)} \) commute with the parity operators \( \Pi_{1,2,3} \):

\[ [\hat{\mathcal{C}}_{\text{grav}}^{(\mu)'}, \Pi_I] = 0, \quad [\hat{\mathcal{C}}_{\text{grav}}^{(\mu)}, \Pi_I] = 0, \quad (8.14) \]
where \( \Pi_1|\vec{v}\rangle = |-v_1, v_2, v_3\rangle \) (or equivalently, \( \Pi_1|\vec{\mu}\rangle = |-\mu_1, \mu_2, \mu_3\rangle \)) and so on, which flip the orientation of the triad.

Note that, unlike \( \mathcal{C}^{(\mu)}_{\text{grav}} \) and \( \hat{\mathcal{C}}^{(\mu)}_{\text{grav}} \), because of the presence of nonconstant \( \hat{\mu}_I \) in (8.9) and (8.10), the operators \( \hat{\mathcal{C}}^{(\mu)}_{\text{grav}} \) and \( \mathcal{C}^{(\mu)}_{\text{grav}} \) are not self-adjoint in \( \mathcal{H}^S_{\text{grav}} \), unless further re-ordering is performed. Nevertheless, the operator \( \Theta \) to be defined in (8.21) is self-adjoint in \( L^2(\mathbb{R}^3_{\text{Bohr}}, B(\vec{v})d^3v_{\text{Bohr}}) \) with proper measure \( \tilde{B}(\vec{v}) \) chosen. Therefore, the procedures used in \( \gamma\mu \)-scheme to construct the physical sector can still be applied for the improved scheme. (Also see the remark in Appendix B.2 for the issue of re-ordering in the isotropic case.)

Remark: To impose the “adaptive” regularization, a seemingly direct but in fact misconceived method would be to set \( S^{(\hat{\mu}_1, \hat{\mu}_2)} \) (the rectangular surface normal to the \( z \)-direction with the side lengths \( \bar{\mu}_3 o L_1 \) and \( \bar{\mu}_3 o L_2 \) in \( x \)- and \( y \)-directions) to the smallest area \( \Delta \) and so on for the other two directions. Instead of (8.3), this method gives \( \bar{\mu}_1 = \sqrt{\frac{\mu_1 k}{\mu_2 \mu_3}}, \bar{\mu}_2 = \sqrt{\frac{\mu_2 k}{\mu_1 \mu_3}}, \) and \( \bar{\mu}_3 = \sqrt{\frac{\mu_3 k}{\mu_1 \mu_2}} \), which mingle the three diagonal directions and complicate the Hamiltonian constraint (in particular, the evolution constraint is no longer a difference equation). A more careful consideration urges that we should use the “square” surface \( S^{(\bar{\mu}_3)} \) rather than the generic “rectangular” surface \( S^{(\bar{\mu}_1, \bar{\mu}_2)} \) to reflect the discreteness imprinted from the full theory. In the full theory, the discretized area is associated with the edge of the spin network which penetrates the surface and carries the \( su(2) \) label \( j \). Therefore, in the symmetry reduced theory, to properly impose the discreteness, the role of \( j \) is replaced by the single label \( \bar{\mu}_I \) in the normal direction to describe the area of the associated surface. \( \square \)

B. Inverse Triad Operators and the Total Hamiltonian Constraint

In \( \bar{\mu} \)-scheme, by the same spirit as discussed in the previous subsection, the inverse triad operators defined in (4.15) should be changed as well by replacing \( \gamma \mu \) with \( \bar{\mu}_I \), and correspondingly, when acting on the states, (4.16) is modified as

\[
\left[ \frac{1}{\sqrt{|\bar{\mu}|}} \right] |\vec{v}\rangle = \frac{1}{4\pi\gamma \ell_{\text{Pl}}^2 \bar{\mu}_1} \left| L_{v_I+1} - L_{v_I-1} \right| |\vec{v}\rangle \\
= (4\pi\gamma k)^{-\frac{1}{2}} \ell_{\text{Pl}}^{-1} |v_I|^\frac{1}{2} \left| v_I + 1 \right|^\frac{1}{2} - \left| v_I - 1 \right|^\frac{1}{2} |\vec{v}\rangle,
\]

where \( L_I \) is the eigenvalue of the length operators:

\[
L_I = (4\pi\gamma)^{1/2} \left( \frac{3\sqrt{k}}{2} \right)^{1/3} |v_I|^{1/3} \ell_{\text{Pl}}.
\]

Note that as in \( \gamma\mu \)-scheme, the inverse triad operators in \( \bar{\mu} \)-scheme commute with \( \hat{p}_I \) and are self-adjoint in \( \mathcal{H}^S_{\text{grav}} \) and bounded above as well. The upper bound is given at \( v_I = \pm 1 \):

\[
|\hat{p}_I|_{\text{max}}^{-\frac{1}{2}} = 2^{1/3} (4\pi\gamma k)^{-1/2} \ell_{\text{Pl}}^{-1}.
\]

\( ^{11} \) The author thanks Ashtekar and Pawlowski for clarifying this confusion.
Furthermore, the eigenvalue of $\sqrt{\mu_1}$ goes to zero when $\mu_1 \to 0$ and this fact is important for the resolution of the singularity as discussed in Section IV C.

Since $C_\phi = 8\pi G p_0^2/\sqrt{p_1 p_2 p_3}$ in (3.22), the corresponding operator $\hat{C}_\phi^{(\hat{\mu})}$ acting on the states of $\mathcal{H}_{\text{kin}}^{\text{total}} : = \mathcal{H}_{\text{grav}}^S \otimes \mathcal{H}_\phi$ yields

$$\hat{C}_\phi^{(\hat{\mu})} | \vec{v} \rangle \otimes | \phi \rangle = \frac{1}{(4\pi \gamma)^2 \ell_\text{Pl}^3} B(\vec{v}) | \vec{v} \rangle \otimes 8\pi G p_0^2 | \phi \rangle,$$

where

$$B(\vec{v}) := \frac{3\sqrt{k}}{2} \frac{1}{\bar{\mu}_1 \bar{\mu}_2 \bar{\mu}_3} \left| v_1 + 1 \right|^{1/3} - \left| v_1 - 1 \right|^{1/3} \left| v_2 + 1 \right|^{1/3} - \left| v_2 - 1 \right|^{1/3} \left| v_3 + 1 \right|^{1/3} - \left| v_3 - 1 \right|^{1/3} \right| v_1 - 1 \right|^{1/3} - \left| v_2 - 1 \right|^{1/3} \right| v_2 + 1 \right|^{1/3} - \left| v_2 - 1 \right|^{1/3} \right| v_3 + 1 \right|^{1/3} - \left| v_3 - 1 \right|^{1/3} \right| v_1 - 1 \right|^{1/3} - \left| v_2 - 1 \right|^{1/3} \right| v_2 + 1 \right|^{1/3} - \left| v_2 - 1 \right|^{1/3} \right| v_3 + 1 \right|^{1/3} - \left| v_3 - 1 \right|^{1/3}. \quad (8.19)$$

The total Hamiltonian constraint $\hat{C}_{\text{grav}}^{(\hat{\mu})} + \hat{C}_\phi^{(\hat{\mu})} = 0$ then gives

$$8\pi G B(\vec{v}) p_0^2 | \vec{v}, \phi \rangle + (4\pi \gamma)^2 \ell_\text{Pl}^3 \hat{C}_{\text{grav}}^{(\hat{\mu})} | \vec{v}, \phi \rangle = 0. \quad (8.20)$$

Again, we choose the standard Schrödinger representation for $\phi$ but the “polymer representation” for $\vec{v}$ (or equivalently for $\vec{\mu}$); that is $\mathcal{H}_{\text{kin}}^{\text{total}} = L^2(\mathbb{R}_\text{Bohr}^3, d^3 v_\text{Bohr}) \otimes L^2(\mathbb{R}, d\phi)$. In this representation, $\hat{p}_\phi = \hbar \frac{\partial}{\partial \phi}$ and the total Hamiltonian constraint read as

$$\frac{\partial^2}{\partial \phi^2} \Psi(\vec{v}, \phi) = \pi G \left[ \tilde{B}(\vec{v}) \right]^{-1} \left\{ C_3^{++}(\vec{v}) \Psi(v_1 + 2, v_2 + 2, v_3, \phi) - C_3^{-+}(\vec{v}) \Psi(v_1 - 2, v_2 + 2, v_3, \phi) \right.$$

$$\left. - C_3^{+-}(\vec{v}) \Psi(v_1 + 2, v_2 - 2, v_3, \phi) + C_3^{--}(\vec{v}) \Psi(v_1 - 2, v_2 - 2, v_3, \phi) \right\} + \text{cyclic terms}$$

$$=: - (\Theta_3(v_1, v_2) + \Theta_2(v_1, v_3) + \Theta_1(v_2, v_3)) \Psi(\vec{v}, \phi) =: - \Theta(\vec{v}) \Psi(\vec{v}, \phi), \quad (8.21)$$

where we define

$$\tilde{B}(\vec{v}) := \bar{\mu}_1 \bar{\mu}_2 \bar{\mu}_3 B(\vec{v})$$

$$= \frac{3\sqrt{k}}{2} \left| v_1 + 1 \right|^{1/3} - \left| v_1 - 1 \right|^{1/3} \left| v_2 + 1 \right|^{1/3} - \left| v_2 - 1 \right|^{1/3} \left| v_3 + 1 \right|^{1/3} - \left| v_3 - 1 \right|^{1/3}. \quad (8.22)$$

By inspection, we can easily see that $\Theta$ and each of $\Theta_{1,2,3}$ individually are self-adjoint on $L^2(\mathbb{R}_\text{Bohr}^3, \tilde{B}(\vec{v}) d^3 v_\text{Bohr})$.

**Note:** The total Hamiltonian constraint in $\vec{\mu}$-scheme for the isotropic case can be obtained by formally “translating” the anisotropic results found in this section. This is shown in Appendix B 2 where the different factor orderings for $\hat{C}_{\text{WDW}}^{(\hat{\mu})}$ and $\hat{C}_{\text{grav}}^{(\hat{\mu})}$ used in this paper and in [8] are also remarked.
C. WDW Theory (Revisited)

When the improved dynamics (\(\tilde{\mu}\)-scheme) is adopted in LQC, the corresponding WDW theory remains the same. In order to compare the WDW theory with LQC in the new scheme, we recast the results in Section VI in terms of the affine variables \(v_I\) defined in (8.3). This change of variables is straightforward and we only list the results.

The total WDW Hamiltonian constraint in (6.3) becomes

\[
\frac{\partial^2 \Psi}{\partial \phi^2} = \frac{\partial}{\partial v} \left( \frac{3\sqrt{k}}{2} \right)^{\frac{3}{2}} \frac{\text{sgn}(v_1v_2)}{|v_3|^{1/3}} \left( |v_2|^{\frac{3}{2}} |v_1|^{\frac{3}{2}} \right) \frac{\partial \Psi}{\partial v_2} + |v_1|^{\frac{3}{2}} \left( |v_1|^{\frac{3}{2}} |v_2|^{\frac{3}{2}} \right) \frac{\partial \Psi}{\partial v_1}
\]

+ cyclic terms\}

\[
= 8\pi G \left[ B(\tilde{v}) \right]^{-1} \left\{ \left( \frac{3\sqrt{k}}{2} \right)^{\frac{3}{2}} \frac{\text{sgn}(v_1v_2)}{|v_3|^{1/3}} \left( |v_2|^{\frac{3}{2}} |v_1|^{\frac{3}{2}} \right) \frac{\partial \Psi}{\partial v_2} + |v_1|^{\frac{3}{2}} \left( |v_1|^{\frac{3}{2}} |v_2|^{\frac{3}{2}} \right) \frac{\partial \Psi}{\partial v_1} \right\} \Psi
\]

\[
= - (\Theta_1(v_1, v_2) + \Theta_2(v_1, v_3) + \Theta_3(v_1, v_3)) \Psi = -\Theta(v) \Psi,
\]

where \(B(\tilde{v}) = B(\tilde{\mu}) = (3\sqrt{k}/2)^{-1} |v_1v_2v_3|^{-1/3}\) and we also define

\[
\tilde{B}(\tilde{v}) := \left( \frac{2}{3} \right)^{3} \left( \frac{3\sqrt{k}}{2} \right)^{2} |v_1v_2v_3|^{-1/3} \tilde{B}(\tilde{v}) = \left( \frac{2}{3} \right)^{3} \left( \frac{3\sqrt{k}}{2} \right)^{2} |v_1v_2v_3|^{-2/3},
\]

which gives

\[
\frac{\partial^2 \Psi}{\partial \phi^2} = \tilde{B}(\tilde{v}) \Psi.
\]

Note that in LQC theory, \(B(\tilde{v})\) and \(\tilde{B}(\tilde{v})\) defined in (8.19) and (8.22) give the expected asymptotic behaviors: \(B(\tilde{v}) \rightarrow B(\tilde{\omega})\) and \(\tilde{B}(\tilde{v}) \rightarrow \tilde{B}(\tilde{\omega})\) when \(|v_1,2,3| \gg 1\).

The operators \(\Theta\) and each of \(\Theta_1,2,3\) individually are self-adjoint on \(L^2(\mathbb{R}^3, B(\tilde{v}) d^3v)\). The (symmetric) eigenfunctions of \(\Theta\) in (6.4) now read as

\[
\xi_k(\tilde{v}) = \xi_k(\tilde{\mu}) = \frac{(3\sqrt{k}/2)^{-\frac{1}{2}} e^{i\frac{\pi}{4}(k_1+k_2+k_3)}}{(4\pi)^3} |v_1v_2v_3|^{-\frac{k}{2}} e^{i\frac{\pi}{4}k_1|v_1|} e^{i\frac{\pi}{4}k_2|v_2|} e^{i\frac{\pi}{4}k_3|v_3|}.
\]

The corresponding eigenvalues are unchanged and given by (6.5). The orthonormality relation (6.6) is rewritten as

\[
\int d^3v \tilde{B}(\tilde{v}) \xi_k^*(\tilde{v}) \xi_{k'}^*(\tilde{v}) = \delta^3(\tilde{k}, \tilde{k}'),
\]

and the completeness relation (6.7) gives

\[
\int d^3v \tilde{B}(\tilde{v}) \xi_k^*(\tilde{v}) \Psi(\tilde{v}) = 0 \quad \text{for } \forall \tilde{k}, \quad \text{iff } \Psi(\tilde{v}) = 0
\]
for any $\Psi(\vec{v}) \in L^2_{\text{phy}}(\mathbb{R}^3, \tilde{B}(\vec{v}) \, d^3 v)$.

The complete set of Dirac observables is comprised of $\hat{p}_\phi$ and $\hat{v}_{\phi_o} (\hat{v} \text{ at some particular instant } \phi = \phi_o)$. The representation of the Dirac observables on $\mathcal{H}_{\text{phy}}^{\text{WDW}}$ is given by (cf. (6.16)):

$$\overline{v_I|_{\phi_o}} \Psi(\vec{v}, \phi) = e^{i\sqrt{\Theta_o}(\phi-\phi_o)}|v_I\rangle \Psi(\vec{v}, \phi_o) \quad \text{and} \quad \hat{p}_\phi \Psi(\vec{v}, \phi) = \hbar \sqrt{\Theta_o} \Psi(\vec{v}, \phi).$$  \hspace{1cm} (8.29)

Both $\hat{p}_\phi$ and $\overline{v}_{\phi_o}$ are self-adjoint on the physical Hilbert space $\mathcal{H}_{\text{phy}}^{\text{WDW}}$ endowed with the inner product (cf. (6.15)):

$$\langle \Psi_1 | \Psi_2 \rangle_{\text{phy}} = \int d^3 v \, \tilde{B}(\vec{v}) \overline{\Psi_1(\vec{v}, \phi_o)} \Psi_2(\vec{v}, \phi_o).$$ \hspace{1cm} (8.30)

The semi-classical (coherent) states are the same as discussed in Section VI C. The approximations used here are valid if the semi-classical states are sharply peaked at the classical values.

The WDW theory recast in terms of the affine variables gives us the asymptotic behavior ($|v_{1,2,3}| \gg 1$) of the general solutions and the physical sector of LQC, which will be discussed in the next subsection.

D. Emergent Time, General Solutions and the Physical Sector

Just like the Hamiltonian equation (7.5) in $\mu$-scheme, the improved Hamiltonian equation (8.21) in $\tilde{\mu}$-scheme has the similar structure. All the results studied in Section VII B – Section VII D can be easily reproduced and modified for the $\tilde{\mu}$-scheme in the obvious manner (using the affine variables $v_I$). Again, (8.21) can be regarded as an evolution equation with respect to the emergent time $\phi$ and the $\phi$-independent operator $\Theta(\vec{v})$ is a difference operator.

The space of physical states is naturally divided into sectors, each of which is preserved by the evolution and by the action of the Dirac observables. This again implies the super-selection for different sectors. Let $\mathcal{L}_{|\epsilon_I|}$ ($|\epsilon_I| \leq 1$) be the “lattice” of points $\{|\epsilon_I| + 2n; n \in \mathbb{Z} \}$ on the $v_I$-axis, $\mathcal{L}_{-|\epsilon_I|}$ be the “lattice” of points $\{-|\epsilon_I| + 2n; n \in \mathbb{Z} \}$ and $\mathcal{L}_{\epsilon_I} = \mathcal{L}_{|\epsilon_I|} \cup \mathcal{L}_{-|\epsilon_I|}$. Also let $\mathcal{H}_{\text{phys}}^{\text{grav}}$ denote the physical subspace of $L^2(\mathbb{R}^3_{\text{Bohr}}, \tilde{B}(\vec{v}) \, d^3 v_{\text{Bohr}})$ with states whose support is restricted to the lattices $\mathcal{L}_{|\epsilon_I|} \otimes \mathcal{L}_{|\epsilon_I|} \otimes \mathcal{L}_{|\epsilon_I|}$ and $\mathcal{L}_{\epsilon_I} \otimes \mathcal{L}_{\epsilon_I} \otimes \mathcal{L}_{\epsilon_I}$ respectively. Each of these subspaces is mapped to
itself by $\Theta$. Furthermore, since $\hat{C}^{(\bar{\mu})}$ is self-adjoint on $\mathcal{H}_{\text{grav}}^\text{kin} = L^2(\mathbb{R}^3_{\text{Bohr}}, dq^3 v_{\text{Bohr}})$, it follows that $\Theta$ is self-adjoint on all these physical Hilbert subspaces.

As in the $\gamma\mu$-scheme, since $\mathcal{L}_{\epsilon}$ and $\mathcal{L}_{1\epsilon}$ are mapped to each other by the operator $\Pi_I$, we restrict ourselves to the symmetric sector (i.e., the subspace of $\mathcal{H}_{\text{grav}}^\text{grav}$ in which $\Psi(\bar{v}) = \Psi(-v_1, v_2, v_3) = \Psi(v_1, -v_2, v_3) = \Psi(v_1, v_2, -v_3)$).

For a generic $\bar{\epsilon}$ (i.e., none of $\epsilon_i$ equals to 0 or 1), we can solve for the eigenvalue equation $\Theta e_\lambda(\bar{v}) = (\Theta_1 + \Theta_2 + \Theta_3) e_\lambda(\bar{v}) = \lambda e_\lambda(\bar{v})$ on each of the 8 Hilbert space $\mathcal{H}_{\epsilon}^\text{grav}$. Let $e_\lambda(v_1, v_2, v_3) = e_{\lambda_1}(v_1) e_{\lambda_2}(v_2) e_{\lambda_3}(v_3)$ and solve (cf. (7.13)):

$$\Theta_3 e_{\lambda_3}(v_1, v_2) = \lambda_{12} e_{\lambda_2}(v_1, v_2), \quad \text{for } e_{\lambda_3}(v_1, v_2) = e_{\lambda_1}(v_1) e_{\lambda_2}(v_2),$$

$$\Theta_2 e_{\lambda_2}(v_1, v_3) = \lambda_{13} e_{\lambda_3}(v_1, v_3), \quad \text{for } e_{\lambda_2}(v_1, v_3) = e_{\lambda_1}(v_1) e_{\lambda_3}(v_3),$$

$$\Theta_1 e_{\lambda_1}(v_2, v_3) = \lambda_{23} e_{\lambda_3}(v_2, v_3), \quad \text{for } e_{\lambda_1}(v_2, v_3) = e_{\lambda_2}(v_2) e_{\lambda_3}(v_3),$$

(8.33)

with $\lambda = \lambda_{12} + \lambda_{13} + \lambda_{23}$. (Note that $\Theta_J$ is independent of $v_I$.) Each of (8.33) can be solved recursively for any arbitrary $\lambda_J$ provided that the appropriate boundary condition is given. For example, $\Theta_3 e_{\lambda_3}(v_1, v_2) = \lambda_{12} e_{\lambda_2}(v_1, v_2)$ reads as (cf. (7.14)):

$$\tilde{C}_I^{\pm \pm}(v_2) e_{\lambda_2}(v_2) = \lambda_{12} e_{\lambda_2}(v_1, v_2) - \tilde{C}_I^{\pm \pm}(v_2) e_{\lambda_2}(v_1, v_2) \lambda_{12}$$

$$\tilde{C}_I^{\pm \pm}(v_2) e_{\lambda_2}(v_1, v_2) = e_{\lambda_2}(v_1, v_2) \lambda_{12}$$

(8.34)

where we define

$$\tilde{C}_I^{\pm \pm}(v, k_J) := \frac{\pi G}{2} [\tilde{B}(\bar{v})]^{-1} C_I^{\pm \pm}(v),$$

(8.35)

which is independent of $\mu_I$ and has the same properties as $\tilde{C}_I^{\pm \pm}(\mu_J, \mu_K)$ does in (7.10) - (7.12). Since the coefficients $\tilde{C}_I^{\pm \pm}$ never vanish or go to infinity on the generic lattice, $e_{\lambda_2}(v_1, v_2)$ can be obtained for any $\lambda_2$ when the values of $e_{\lambda_3}(v_1 + 2, v_2 + 2)$, $e_{\lambda_3}(v_1, v_2)$ and $e_{\lambda_2}(v_1, v_2)$ are given. As a result, if the values of $e_{\lambda_3}(v_1, v_2)$ are specified on the boundary lines $v_1 = v_1$, $v_1 = v_1 - 2$ and $v_2 = v_2$, $v_2 = v_2 - 2$ in the lattice $\mathcal{L}_{\epsilon}$, $e_{\lambda_2}(v_1, v_2)$ can be uniquely determined via the recursion relation (8.34) for all the lattice points with $v_1 < v_1$ and $v_2 < v_2$.

On the other hand, the LQC operator $\Theta_J$ reduces to the WDW operator $\Theta_J$ in the asymptotic regime (i.e., $|v_J| \gg 1$), and thus the LQC eigenfunction $e_\epsilon(\bar{v})$ approaches the WDW eigenfunction $e_\epsilon(\bar{v})$ given by (8.26) for large $|v_J|$. Therefore, we can use the same labels $k_i$ to denote the LQC eigenfunctions (i.e., $\lambda_{1,2,3} = k_{1,2,3}$) and similarly decompose $e_\epsilon(\bar{v})$ as $e_{k_i}(v_1) e_{k_2}(v_2) e_{k_3}(v_3)$. It follows that $e_{k_i}(v_I) \to e_{k_i}(v_I)$ for $|v_I| \gg 1$ and we have the identifications (7.13) and (8.16) unchanged. Again, the LQC operator $\Theta$ is not positive definite and only those modes with $\omega^2 > 0$ are allowed. What matters is the operator $\Theta_+$, obtained by projecting the action of $\Theta$ to the positive eigenspace in its spectral decomposition.

For a given $\vec{k}$, $e_{\lambda_J}$ can be obtained as mentioned above by appropriately specifying the boundaries in such a way that $e_{\lambda_J}(v_1, v_J) \to e_{k_i}(v_1) e_{k_i}(v_J)$ for $|v_I| \gg 1$, $|v_J| \gg 1$. To be used for the boundary condition, however, the asymptotic function $e_{k_i}(v_1) e_{k_i}(v_2)$ is given by (8.26) should be further “tamed”. Following the same spirit used for $\gamma\mu$-scheme, the value of $e_{\lambda_2}(\mu_1, \mu_2)$ on the boundary is given by (cf. (7.17)):

$$\left(\frac{3\sqrt{k}/2}{(4\pi)^2}\frac{3}{2} \left|v_1 + 1\right|^{\frac{1}{3}} - \left|v_1 - 1\right|^{\frac{1}{3}}\right)^{\frac{1}{2} - ik_1} \times \left(\frac{3}{2} \left|v_2 + 1\right|^{\frac{1}{3}} - \left|v_2 - 1\right|^{\frac{1}{3}}\right)^{\frac{1}{2} - ik_2},$$

(8.36)
which again reduces to \( e^{-\lambda}(v_1) e^{-\lambda}(v_2) \) when both \(|v_1| \gg 1\) and \(|v_2| \gg 1\). In practice, we use (8.36) to specify the boundary condition on the lines \((v_1 = v_1^*, -v_2^* \leq v_2 \leq v_2^*)\), \((v_1 = v_1^* - 2, -v_2^* \leq v_2 \leq v_2^*)\), \((-v_1^* \leq v_1 \leq v_1^*, v_2 = v_2^*)\) and \((-v_1^* \leq v_1 \leq v_1^*, v_2 = v_2^* - 2)\) of the lattice for \(v_1^* \gg 1\) and \(v_2^* \gg 1\), then the recursion relation (8.34) uniquely gives the values \(e_{\lambda,j}(v_1, v_2)\) for all the lattice points within the range \(-v_1^* \leq v_1 \leq v_1^*\) and \(-v_2^* \leq v_2 \leq v_2^*\).

Similarly, all the other results and remarks in Section VII B – Section VII D can be easily modified for the \(\bar{\mu}\)-scheme by formally taking the replacements: \(\mu_I \rightarrow v_I\) and \(\bar{B}(\bar{\mu}) \rightarrow \bar{B}(\bar{v})\). In particular, the orthonormality relation for the eigenfunctions in the symmetric sector of \(H_{e,grav}^\text{sym}\) is given by (cf. (7.19)):

\[
\sum_{\bar{v} \in L_{v_1} \otimes L_{v_2} \otimes L_{v_3}} \bar{B}(\bar{v}) \tilde{e}^{(s)}_{\bar{k}}(\bar{v}) e^{(s)}_{\bar{k}'}(\bar{v}) = \delta^{3}(\bar{k}, \bar{k}')
\]

and the completeness relation reads as (cf. (7.20)):

\[
\sum_{\bar{v} \in L_{v_1} \otimes L_{v_2} \otimes L_{v_3}} \bar{B}(\bar{v}) \tilde{e}^{(s)}_{\bar{k}}(\bar{v}) \Psi(\bar{v}) = 0 \quad \text{for } \forall \bar{k}, \quad \text{iff } \Psi(\bar{v}) = 0
\]

for any symmetric \(\Psi(\bar{v}) \in H_{e,grav}^\text{sym}\). The general symmetric solution to the improved LQC constraint (8.21) can be written as (cf. (7.22)):

\[
\Psi(\bar{v}, \phi) = \int d^3k \left( \tilde{\Psi}_+(\bar{k}) \tilde{e}^{(s)}_{\bar{k}}(\bar{v}) e^{i\omega\phi} + \tilde{\Psi}_-(\bar{k}) \tilde{e}^{(s)}_{\bar{k}}(\bar{v}) e^{-i\omega\phi} \right)
\]

where \(\tilde{\Psi}_\pm(\bar{k})\) are in \(L^2(\mathbb{R}^3, d^3k)\). The solution to (8.21) with the “initial” function \(\Psi_\pm(\bar{v}, \phi_0) = f_\pm(\bar{v})\) is (cf. (7.24)):

\[
\Psi_\pm(\bar{v}, \phi) = e^{\pm i/\sqrt{\Theta_+}(\phi-\phi_0)} \Psi_\pm(\bar{v}, \phi_0),
\]

where \(\sqrt{\Theta_+}\) is the square-root of the positive self-adjoint operator \(\Theta_+\) defined via spectral decomposition.

Finally, the super-selection sector of the physical Hilbert space \(H_{e,phy}^\text{sym}\) labeled by \(\bar{e} \in [0, 1] \times [0, 1] \times [0, 1]\) consists of the positive frequency solutions \(\Psi(\bar{v}, \phi)\) to (8.21) with initial data \(\Psi(\bar{v}, \phi_0)\) in the symmetric sector of \(H_{e,grav}^\text{sym}\). By (8.39), the explicit expression in terms of the symmetric eigenfunctions \(e^{(s)}_{\bar{k}}\) is given by (cf. (7.30)):

\[
\Psi(\bar{v}, \phi) = \int d^3k \tilde{\Psi}(\bar{k}) \tilde{e}^{(s)}_{\bar{k}}(\bar{v}) e^{i\omega\phi},
\]

where \(\omega^2(\bar{k}) = 16\pi G(k_1k_2 + k_1k_3 + k_2k_3 + 3/16)\). The physical inner product on the physical sector \(H_{e,phys}^\text{sym}\) is given by (cf. (7.31)):

\[
\langle \Psi_1 | \Psi_2 \rangle_{e,phys} = \sum_{\bar{v} \in L_{v_1} \otimes L_{v_2} \otimes L_{v_3}} \bar{B}(\bar{v}) \tilde{\Psi}_1(\bar{v}, \phi_0) \tilde{\Psi}_2(\bar{v}, \phi_0).
\]

The action of the Dirac observables is independent of \(\bar{e}\) and has the same form as in the WDW theory (cf. (7.32)):

\[
\hat{v}_I|\phi_0\rangle \Psi(\bar{v}, \phi) = e^{i/\sqrt{\Theta_+}(\phi-\phi_0)}|v_I\rangle \Psi(\bar{v}, \phi_0) \quad \text{and} \quad \hat{p}_\phi \Psi(\bar{v}, \phi) = -i\hbar \frac{\partial \Psi(\bar{v}, \phi)}{\partial \phi}.
\]
Just like the case in $\gamma\mu$-scheme, because of super-selection, each physical sector $\mathcal{H}_\text{phy}$ is separable while the kinematical Hilbert space $\mathcal{H}_\text{kin}^{\text{total}}$ is not. The standard type of discreteness of the Dirac observables $\hat{v}_I|\phi_o$ on each physical sector is descended from the more delicate discreteness of the spectrum of $\hat{v}_I$ on $\mathcal{H}_\text{grav}^{\text{kin}} = L^2(\mathbb{R}^3_{\text{Bohr}}, d^3v_{\text{Bohr}})$.

Finally, it is easy to check that the coefficients $C^{\pm\pm}_I(\vec{v})$ and $\tilde{C}^{\pm\pm}(v_J, v_K)$ have the properties exactly the same as those of $C^{\pm\pm}(\vec{\mu})$ and $\tilde{C}^{\pm\pm}(\mu_J, \mu_K)$ listed in (7.7), (7.8) and (7.10)–(7.12). Together with the fact that $\tilde{B}(0, v_2, v_3) = \tilde{B}(v_1, 0, v_3) = \tilde{B}(v_1, v_2, 0) = 0$, the argument used in Section VII C can be applied to prove the resolution of the classical singularity in $\bar{\mu}$-scheme and to suggest the occurrence of the big bounce. Moreover, by the lesson learned in [8], in $\bar{\mu}$-scheme, the bounces are expected to happen when the directional factor $\bar{g}_I := p^2_\phi / |\bar{p}_I|^3$ enters the Planck regime of $O(\hbar \ell_P^{-3})$, independent of the values of $p_\phi$.

Meanwhile, the planar collapse is not resolved but persists in $\bar{\mu}$-scheme, yielding the same comments as made in the end of Section VII C.

IX. DISCUSSION

The analytical investigation in this paper is the direct extension of [1] and [8], developing a comprehensive LQC framework for the anisotropic Bianchi I model. Both the precursor ($\gamma\mu$-) and the improved ($\bar{\mu}$-) strategies are successfully deployed. The key features responsible for the desired results remain the same: (i) the kinematical framework of LQC forces us to replace the connection variables by the holonomies, and (ii) the underlying quantum geometry gives rise to the discreteness in the spectrum of the triad operators, as the imprint of the fundamental “area gap” in the full theory. Furthermore, following the $\bar{\mu}$-scheme newly proposed in [8], a more sophisticated prescription is introduced to impose the discreteness, thereby capturing the underlying physics of quantum geometry in a more sensible way.

The success of this extension affirms the robustness of the methods in [1, 8] and thus enlarges their domain of validity. It also shows the fact that the singularity persists in the WDW theory is rather generic, even in the less symmetric model. The main difference with anisotropy is that the operator $\Theta$ is no longer positive definite. Nevertheless, the detailed analysis shows that the only relevant part is $\Theta_+ \Theta_+$ (the projection of $\Theta$ on its positive eigenspace) and therefore the strategies can be readily carried through without a big modification. Consequently, the expected results for the Bianchi I model are established: (i) the scalar field $\phi$ again serves as an internal clock and is treated as emergent time; (ii) the total Hamiltonian constraint is derived in both $\gamma\mu$- and $\bar{\mu}$-schemes and gives the evolution as a difference equation; and (iii) the physical Hilbert space, Dirac observables and semi-classical states are constructed rigorously.

On the other hand, the variety of anisotropy does give new features, notably distinct from those in isotropic models. Unlike the isotropic case, the Bianchi I model with a massless scalar field admits both Kasner-like and Kasner-unlike solutions in the classical dynamics. In the quantum theory, we anticipate that the singularity (both Kasner-like and Kasner-unlike) is resolved. This is evidenced by the observation: in the kinematical Hilbert space, the state associated with the classical singularity is completely decoupled from the other states in the difference evolution equation, and therefore the evolution is deterministic across the deep Planck regime.

Meanwhile, we have the somewhat surprising observation that the planar collapse for Kasner-like solutions is not resolved and thus the vanishing behavior of the length scale
factors $a_I$ is not prevented by the quantum effect. This suggests that either area is more fundamental than length in LQG or some important ingredient is missing when we impose the discreteness correction from the full theory. Either case requires further studies.

To actually figure out the behaviors of the quantum evolution, the analytical investigation alone is not enough. A complete numerical analysis or at least the study of effective dynamics is in demand \[11,12\]. We expect that the big bounce occurs whenever one of the area scales $p_I$ undergoes the vanishing behavior. It may happen as many as three times. Furthermore, in the improved dynamics ($\bar{\mu}$-scheme), the bounce takes place at the moment when the directional factor $q_I$ in any of the three diagonal directions comes close to the critical value in the Planck regime, regardless of the values of $p_\phi$.

Other possible extensions have been discussed and commented in Discussion of [1]. In particular, in order to understand the BKL scenario in the context of LQC, the next step would be to explore Bianchi IX models based on the same formulation. Meanwhile, as both the isotropic and Bianchi I models have been analyzed in great detail, another feasible research direction is to study the emergence of isotropy in the arena of Bianchi I models, which could shed some light on the symmetry reduction for more complicated situations.

As remarked in the end of Appendix B1, this issue is not trivial and demands more detailed investigation.

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APPENDIX A: WDW SEMI-CLASSICAL (COHERENT) STATES

In this appendix, we study more details about the WDW semi-classical states described in Section VI C. We first look closer at the semi-classical state to better understand its structure and then compute the physical quantities corresponding to the Dirac observables.

The semi-classical states in WDW theory are constructed in (6.17) with $\tilde{\Psi}(\vec{k})$ sharply peaked at $\vec{k} = K\vec{\kappa}$. Since $\tilde{\Psi}(\vec{k})$ is sharply distributed, only those $\vec{k}$ close to $K\vec{\kappa}$ contribute. For $K\kappa_\phi \gg 1$, $\omega^2(\vec{k}) \approx 16\pi G(k_1k_2 + k_1k_3 + k_2k_3) \approx 8\pi Gk^2\kappa^2_\phi$ in the vicinity of $\vec{k} = K\vec{\kappa}$. As a result, the physical condition $\omega^2 > 0$ is automatically satisfied for the relevant $\vec{k}$. Therefore, when a sharply-peaked semi-classical state is concerned, the restriction $\omega^2 > 0$ for the integral range in (6.17) can be ignored. We will make use of this fact to simplify the following calculations.

With the inner product defined in (6.15), we have

$$\langle \tilde{\Psi}(\vec{k}) | \tilde{\Psi}(\vec{k}') \rangle_{\text{phy}} = \int \frac{d^3k \cdot d^3k'}{\omega^2(\vec{k})\omega^2(\vec{k}') > 0} \delta^3(\vec{k}, \vec{k}') \tilde{\Psi}(\vec{k}') \bar{\Psi}(\vec{k}) e^{i(\omega(\vec{k}) - \omega(\vec{k}'))(\phi_0 - \phi',\phi_0')},$$

$$\approx \frac{1}{(2\pi)^3/2\sigma_1\sigma_2\sigma_3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dk_1dk_2dk_3 e^{-\frac{(k_1 - K\kappa_1)^2}{2\sigma_1^2}} e^{-\frac{(k_2 - K\kappa_2)^2}{2\sigma_2^2}} e^{-\frac{(k_3 - K\kappa_3)^2}{2\sigma_3^2}} = 1, \quad (A1)$$
where the identity (6.16) is used and the restriction \( \omega^2 > 0 \) is released. The overall factors in (6.18) has been chosen to make the physical norm of the state normalized.

Before computing the expectation value and dispersion for \( \hat{\mu}_{\phi_o} \), first note that by \( e^{ia \hat{f}} f(x) = f(x+a) \) and (6.4) we have
\[
e^{-\frac{i \omega}{\hbar} \hat{\epsilon}_k(\mu)} = |\mu_1|^a \hat{\epsilon}_k(\mu) \tag{A2}
\]
and consequently
\[
\int d^3 \mu B(\mu) \hat{\epsilon}_k(\mu) |\mu_1|^a \hat{\epsilon}_k(\mu) = e^{-\frac{i \omega}{\hbar} \hat{\epsilon}_k(\mu)} \delta^3(\vec{k}, \vec{k}'). \tag{A3}
\]

The derivatives of \( \delta^3(\vec{k}, \vec{k}') \) can be handled with integral by part. This then leads to
\[
\langle \mu_1 | \phi_o \rangle := \langle \Psi_{\mu_o} | \hat{\mu}_o \Psi_{\mu_o} \rangle_{\text{phys}} \\
\approx \int d^3 k d^3 k' \delta^3(\vec{k}, \vec{k}') \tilde{\Psi}_k(\vec{k}) e^{-i \omega(\vec{k}) (\phi_o - \phi_o')} e^{i \frac{\omega}{\hbar} (\vec{k}) (\phi_o - \phi_o')} \tag{A4}
\]
Applying \( e^{ia \hat{f}} f(x) = f(x+a) \) again, we have (taking \( I = 1 \))
\[
e^{\frac{2a}{(2\pi)^2}} e^{\frac{\omega}{\hbar} (\vec{k}) (\phi_o - \phi_o')} = e^{\frac{2a}{(2\pi)^2}} e^{\frac{\omega}{\hbar} (\vec{k}) (\phi_o - \phi_o')}
\]
where in the second line, we simply assign the peaked value to the integrand. This is the result in (6.21).

Similarly, taking \( \alpha = 2 \) in (A2) and following the same procedure, we have
\[
\langle \mu_1 | \phi_o \rangle^2 \approx \int d^3 k e^{\frac{2a}{(2\pi)^2}} e^{\frac{\omega}{\hbar} (\vec{k}) (\phi_o - \phi_o')} \tilde{\Psi}_k(\vec{k}) \tilde{\Psi}_k(\vec{k})
\]
which leads to the variance in (6.22).

Next, to compute the expectation value for \( p_\phi \), we recall the action of \( \hat{p}_\phi \) defined in (6.14) and use the fact \( \sqrt{\bar{\epsilon}_k(\mu)} = \omega(\vec{k}) \hat{\epsilon}_k(\mu) \). It follows
\[
\langle p_\phi \rangle = \int_{\omega(\vec{k}) > 0} d^3 k \omega(\vec{k}) \tilde{\Psi}_k(\vec{k}) \tilde{\Psi}_k(\vec{k}) \approx \hbar \omega(\vec{k}) \int d^3 k \tilde{\Psi}_k(\vec{k}) \tilde{\Psi}_k(\vec{k})
\]
\[
= \hbar \sqrt{8\pi G K_{\phi}} \equiv p_\phi^*, \tag{A8}
\]
where again we ignore the restriction for the integral range and directly put the peaked value to the integrand. This is the result in (6.23).

Following the same procedure, we have

\[ \langle p_\phi^2 \rangle = \int_{\omega(k)>0} d^3k \frac{\omega^2(k) \tilde{\Psi}_R(k) \tilde{\Psi}_R(k)}{2}\]

\[ \approx \frac{16\pi G h^2}{(2\pi)^{3/2} \sigma_1 \sigma_2 \sigma_3} \int d^3k (k_1 k_2 + k_1 k_3 + k_2 k_3) e^{-\frac{(k_1 - K_k_1)^2}{2\sigma_1^2} - \frac{(k_2 - K_k_2)^2}{2\sigma_2^2} - \frac{(k_3 - K_k_3)^2}{2\sigma_3^2}} \]

\[ = 16\pi G h^2 K^2 (\kappa_1 \kappa_2 + \kappa_1 \kappa_3 + \kappa_2 \kappa_3) \equiv p_\phi^2, \quad (A8) \]

which leads to \( \Delta^2(p_\phi) = \langle p_\phi^2 \rangle - \langle p_\phi \rangle^2 = 0 \). However, the vanishing of \( \Delta(p_\phi) \) is artificial, resulting merely from the approximations we have used in (A8) and (A9), which neglect the variation in \( \Delta(p_\phi) \) in the order of \( p_\phi^4 \mathcal{O}((\frac{1}{n^2})^{n \geq 1}) \). In order to recover the correct estimate of \( \Delta(p_\phi) \) for the desired order while keeping the integration tractable, we assume \( \langle p_\phi^2 \rangle \approx \langle p_\phi^4 \rangle^{1/2} \) (based on the assumption that \( \tilde{\Psi}_R(k) \) is sharply peaked) and compute \( \langle p_\phi^4 \rangle \) instead:

\[ \langle p_\phi^4 \rangle = \int_{\omega(k)>0} d^3k \frac{\omega^4(k) \tilde{\Psi}_R(k) \tilde{\Psi}_R(k)}{2}\]

\[ \approx \frac{(16\pi G)^2 h^4}{(2\pi)^{3/2} \sigma_1 \sigma_2 \sigma_3} \int d^3k (k_1 k_2 + k_1 k_3 + k_2 k_3)^2 e^{-\frac{(k_1 - K_k_1)^2}{2\sigma_1^2} - \frac{(k_2 - K_k_2)^2}{2\sigma_2^2} - \frac{(k_3 - K_k_3)^2}{2\sigma_3^2}} \]

\[ = (16\pi G)^2 h^4 \left\{ K^2 (\sigma_1^2 (\kappa_2 + \kappa_3)^2 + \sigma_2^2 (\kappa_1 + \kappa_3)^2 + \sigma_3^2 (\kappa_1 + \kappa_2)^2) \right. \]

\[ + \left. \left( \sigma_1^2 \sigma_2^2 + \sigma_1^2 \sigma_3^2 + \sigma_2^2 \sigma_3^2 \right) + K^4 (\kappa_1 \kappa_2 + \kappa_1 \kappa_3 + \kappa_2 \kappa_3) \right\} \]

\[ \equiv p_\phi^4 \left\{ 1 + \frac{4}{K^2 K^4} (\sigma_1^2 (\kappa_2 + \kappa_3)^2 + \sigma_2^2 (\kappa_1 + \kappa_3)^2 + \sigma_3^2 (\kappa_1 + \kappa_2)^2) \right. \]

\[ + \left. \frac{4}{K^4 K^4} (\sigma_1^2 \sigma_2^2 + \sigma_1^2 \sigma_3^2 + \sigma_2^2 \sigma_3^2) \right\}. \quad (A10) \]

This then gives

\[ \langle p_\phi^2 \rangle \approx \langle p_\phi^4 \rangle^{1/2} = p_\phi^2 \left\{ 1 + \frac{2}{K^2 K^4} (\sigma_1^2 (\kappa_2 + \kappa_3)^2 + \sigma_2^2 (\kappa_1 + \kappa_3)^2 + \sigma_3^2 (\kappa_1 + \kappa_2)^2) \right. \]

\[ + \mathcal{O} \left( \left( \frac{\sigma}{K} \right)^4 \right) \}

\[ \quad + \mathcal{O} \left( \left( \frac{\sigma}{K} \right)^4 \right) \}

\[ \quad + \mathcal{O} \left( \left( \frac{\sigma}{K} \right)^4 \right) \}

and therefore

\[ \Delta^2(p_\phi) = \langle p_\phi^2 \rangle - \langle p_\phi \rangle^2 \approx \frac{2p_\phi^2}{K^2 K^4} (\sigma_1^2 (\kappa_2 + \kappa_3)^2 + \sigma_2^2 (\kappa_1 + \kappa_3)^2 + \sigma_3^2 (\kappa_1 + \kappa_2)^2), \quad (A12) \]

which is the result shown in (6.24).

**APPENDIX B: REMARKS ON THE ISOTROPIC MODEL**

1. **Precursor Strategy (\( \mu_\phi \)-Scheme)**

In this subsection, we discuss how to read off the gravitational constraint operator for the isotropic case from the results obtained in Section \( \text{V A} \) and Section \( \text{V B} \) for the anisotropic cases. In the end, we comment on the symmetry reduction from anisotropy to isotropy.
In the isotropic model, the classical phase space is given by the variables \( c \) and \( p \) with the fundamental Poisson bracket (note the difference of the factor 3):

\[
\{c, p\} = \frac{8\pi \gamma G}{3}.
\]  

(B1)

In quantum kinematics, the eigenstates of \( \hat{p} \) are the basis states \( |\mu\rangle \):

\[
\hat{p}|\mu\rangle = \frac{4\pi \gamma \ell_p^2}{3} |\mu\rangle.
\]  

(B2)

The basis states are also the eigenstates of the volume operator \( \hat{V} \):

\[
\hat{V}|\mu\rangle = V_{\mu}|\mu\rangle := \left( \frac{4\pi \gamma}{3} |\mu| \right)^\frac{2}{3} \ell_p^\frac{3}{2}|\mu\rangle.
\]  

(B3)

To reproduce the isotropic result from the anisotropic Bianchi I models, we can simply take the replacement:

\[
c^1, c^2, c^3 \rightarrow c, \quad p_1, p_2, p_3 \rightarrow p.
\]  

(B4)

In LQC, correspondingly, we take

\[
|\mu_1 + \alpha \gamma \mu_1, \mu_2 + \beta \gamma \mu_2, m_3 + \gamma \mu_3 \rangle \rightarrow |\mu + (\alpha + \beta + \gamma)\mu_0\rangle
\]  

(B5)

and

\[
V_{\mu_1 + \alpha \gamma \mu_1, \mu_2 + \beta \gamma \mu_2, m_3 + \gamma \mu_3} \rightarrow V_{\mu + (\alpha + \beta + \gamma)\mu_0},
\]  

(B6)

where in the end we also impose

\[
\mu_0 = 3 \gamma \mu = 3k \equiv 3\sqrt{3}/2.
\]  

(B7)

The replacement rules then “translate” (5.6) (5.9), (5.10) and (5.7) (5.11) (5.12) to their counterparts in the isotropic model:

\[
\hat{C}^{(\mu_0)}_{\text{grav}, o} = \frac{24i \text{ sgn}(p)}{8\pi \gamma^3 \ell_p^2 \ell_p^3} \left[ \sin^2(\mu_o c) \left( \sin(\frac{\mu_o c}{2})\hat{V} \cos(\frac{\mu_o c}{2}) - \cos(\frac{\mu_o c}{2})\hat{V} \sin(\frac{\mu_o c}{2}) \right) \right],
\]  

(B8)

\[
\hat{C}^{(\mu_0)'} = \frac{1}{2} \left[ \hat{C}^{(\mu_o)}_{\text{grav}, o} + \hat{C}^{(\mu_o)}_{\text{grav}, o} \right],
\]  

(B9)

\[
\hat{C}^{(\mu_0)}_{\text{grav}} = \frac{24i \text{ sgn}(p)}{8\pi \gamma^3 \ell_p^2 \ell_p^3} \left[ \sin(\mu_o c) \left( \sin(\frac{\mu_o c}{2})\hat{V} \cos(\frac{\mu_o c}{2}) - \cos(\frac{\mu_o c}{2})\hat{V} \sin(\frac{\mu_o c}{2}) \right) \right] \sin(\mu_o c)
\]  

(B10)

and

\[
\hat{C}^{(\mu_0)}_{\text{grav}, o}|\mu\rangle = \frac{3}{8\pi \gamma^3 \ell_p^2 \ell_p^3} \left\{ |V_{\mu + \mu_0} - V_{\mu - \mu_0}||\mu + 4\mu_0\rangle - 2|\mu\rangle + |\mu - 4\mu_0\rangle \right\},
\]  

(B11)

\[
\hat{C}^{(\mu_0)'}|\mu\rangle = \frac{3}{16\pi \gamma^3 \ell_p^2 \ell_p^3} \left\{ |V_{\mu + 5\mu_0} - V_{\mu + 3\mu_0}| + |V_{\mu + \mu_0} - V_{\mu - \mu_0}| \right\}|\mu + 4\mu_0\rangle
\]  

\[+\left( |V_{\mu - 3\mu_0} - V_{\mu - 5\mu_0}| + |V_{\mu + \mu_0} - V_{\mu - \mu_0}| \right)|\mu - 4\mu_0\rangle - 4|V_{\mu + \mu_0} - V_{\mu - \mu_0}||\mu\rangle \right\},
\]  

(B12)
\[ C_{grav}^{(\mu_o)} |\mu\rangle = \frac{6}{16\pi^3 \gamma^3 \ell_P^3 \mu_o^3} \left\{ |V_{\mu+3\mu_o} - V_{\mu+\mu_o}| |\mu + 4\mu_o\rangle + |V_{\mu-\mu_o} - V_{\mu-3\mu_o}| |\mu - 4\mu_o\rangle \right. \\
- \left. (|V_{\mu+3\mu_o} - V_{\mu+\mu_o}| + |V_{\mu-\mu_o} - V_{\mu-3\mu_o}|) |\mu\rangle \right\}. \quad (B13) \]

The last one with \( \mu_o = 3k \) is the master equation used in [1].

**Remark:** According to (5.12), the subspace spanned by \( |\mu_1, \mu_2, \mu_3\rangle \) with \( \mu_1 = \mu_2 = \mu_2 \) is not invariant under \( C_{grav}^{(\mu)} \). Hence, by restricting the initial states to the “isotropic sector”, the total Hamiltonian constraint \( C_{grav}^{(\mu)} + C_{\phi}^{(\mu)} = 0 \) does not yield the solution which lays on the isotropic sector for all the time of the evolution. To systematically study how the isotropy appears in the anisotropic framework, more conceptual considerations and technical tools for a better notion of symmetry reduction such as developed in [43, 44] may be needed for the future research. □

### 2. Improved Strategy (\( \bar{\mu} \)-Scheme)

In this subsection, we follow the ideas used in Section VIII A and Section VIII B to construct the total Hamiltonian constraint in \( \bar{\mu} \)-scheme for the isotropic case. In the end, the issue of the different factor orderings for \( \hat{C}_{WDW}^{grav} \) and \( \hat{C}_{grav}^{(\bar{\mu})} \) used in this paper and in [8] are also remarked.

In the isotropic model, the area operator in (4.4) is replaced by

\[ E(S, f) = pV_o^{-\frac{2}{3}} A_{S,f}, \quad (B14) \]

with \( A_{S,f} \) the area of \( S \) measured by \( q_{ab} \) times the factor \( f \). Consider \( S^{(\bar{\mu})} \) to be a square surface with side length \( \bar{\mu}V_o^{-1/3} \) (measured by \( q_{ab} \)), which gives

\[ E(S^{(\bar{\mu})}) |\mu\rangle = p \bar{\mu}^2 |\mu\rangle = \frac{4\pi \gamma^3 \ell_P^2 \bar{\mu}^2 |\mu\rangle}. \quad (B15) \]

When the \( \bar{\mu} \)-scheme is applied to the isotropic case, again, we require the smallest area to be \( 4\pi \gamma^3 \ell_P^2 \bar{\mu}^2 \mu/3 = \pm \Delta \) and thus we set

\[ \bar{\mu} = \sqrt{3k/|\mu|}. \quad (B16) \]

Following the same procedure for the anisotropic case, we solve the affine parameter

\[ \bar{\mu} \frac{\partial}{\partial \mu} := \frac{\partial}{\partial v} \Rightarrow v = \text{sgn}(\mu) \frac{2}{3\sqrt{3k}} |\mu|^{3/2} \quad (B17) \]

and it leads to

\[ e^{\mp \bar{\mu} \frac{\partial}{\partial v}} \psi(\mu) = e^{\mp \frac{\partial}{\partial v}} \psi(v) = \psi(v \mp 1) \quad (B18) \]

or equivalently

\[ e^{\pm \frac{\bar{\mu}c}{2}} |\mu\rangle = |v \pm 1\rangle. \quad (B19) \]

Therefore, (B13) is altered to

\[ \hat{C}_{grav}^{(\bar{\mu})} |v\rangle = \frac{\sqrt{\pi} \ell_P^2}{\sqrt{3} \gamma^2 \bar{\mu}^3} \left\{ C^+(v)|v + 4\rangle + C^-(v)|v - 4\rangle - C^o(v)|v\rangle \right\}. \quad (B20) \]
where
\[ C^+(v) := \frac{3\sqrt{3}k}{2} |v + 3| - |v + 1|, \]
\[ C^-(v) := \frac{3\sqrt{3}k}{2} |v - 1| - |v - 3|, \]
\[ C^o(v) := \frac{3\sqrt{3}k}{2} \left( \left| |v + 3| - |v + 1| \right| + \left| |v - 1| - |v - 3| \right| \right). \]  \tag{B21}

As in the $\mu_o$-scheme shown in Appendix B1, the result of (B20) can be easily obtained from the anisotropic $\hat{C}^{(\tilde{\mu})}_{\text{grav}}$ in (8.10) simply by taking the formal replacements:
\[ |v_1 + \alpha,v_2 + \beta,v_3 + \gamma \rangle \rightarrow |v + (\alpha + \beta + \gamma)\rangle, \]
\[ \tilde{\mu}_{1,2,3} \rightarrow 3^{-1/3} \tilde{\mu} \quad \text{and} \quad V_{v_1 + \alpha,v_2 + \beta,v_3 + \gamma} \rightarrow V_{v + (\alpha + \beta + \gamma)}, \]  \tag{B22}

where $V_v$ is the eigenvalues of the volume operator:
\[ V_v = \left( \frac{4\pi \gamma}{3} \right)^{3/2} \left( \frac{3\sqrt{3}k}{2} \right) |v| \ell_p^3. \]  \tag{B23}

Similarly, the inverse triad operator in the new scheme is given by
\[ \left[ \frac{\text{sgn}(\rho)}{\sqrt{|\rho|}} \right] |v\rangle = \frac{3}{4\pi \gamma \ell_p^3 \bar{\mu}} (V_{v+1}^{1/3} - V_{v-1}^{1/3}) |v\rangle. \]  \tag{B24}

Classically, $C_\phi = 8\pi G \tilde{p}_\phi^2 / |\rho|^{3/2}$ and this is quantized to the LQC operator $\hat{C}^{(\tilde{\mu})}_{\phi}$, which when acting on the states of $\mathcal{H}_{\text{kin}}^{\text{total}}$ yields
\[ \hat{C}^{(\tilde{\mu})}_{\phi} |v\rangle \otimes |\phi\rangle = \left( \frac{3}{4\pi \gamma} \right)^{3/2} \frac{1}{\ell_p^3} B(v) |v\rangle \otimes 8\pi G \tilde{p}_\phi^2 |\phi\rangle \]  \tag{B25}

with
\[ B(v) := \frac{3\sqrt{3}k}{2} \frac{1}{\bar{\mu}^3} \left( |v + 1|^{1/3} - |v - 1|^{1/3} \right)^3. \]  \tag{B26}

Consequently, the total Hamiltonian constraint leads to
\[ \frac{\partial^2}{\partial \phi^2} \psi(v, \phi) = \frac{\pi G}{9} [\bar{B}(v)]^{-1} \left\{ C^+(v) \Psi(v + 4, \phi) + C^-(v) \Psi(v - 4, \phi) - C^o(v) \Psi(v, \phi) \right\} \]
\[ = \frac{\pi G}{9} \left( |v + 1|^{1/3} - |v - 1|^{1/3} \right)^{-3} \]
\[ \times \left\{ |v + 3| - |v + 1| \right| \Psi(v + 4, \phi) + |v - 1| - |v - 3| \right| \Psi(v - 4, \phi) \]
\[ - \left( |v + 3| - |v + 1| \right| + |v - 1| - |v - 3| \right| \Psi(v, \phi) \}
\[ =: \Theta(v) \Psi(v, \phi), \]  \tag{B27}

where we define
\[ \bar{B}(v) := \bar{\mu}^3 B(v) = \frac{3\sqrt{3}k}{2} \left( |v + 1|^{1/3} - |v - 1|^{1/3} \right)^3. \]  \tag{B28}
It can be easily inspected that the operator $\Theta$ is self-adjoint in $L^2(\mathbb{R}_{\text{Bohr}}, \tilde{B}(v) \, dv_{\text{Bohr}})$.

**Remark:** The total Hamiltonian constraint given in (B27) is almost the same as the master equation used in [8]. However, there is a subtle difference. In [8], $\tilde{B}(v)$ is not introduced and the physical Hilbert space is identified as $L^2_S(\mathbb{R}_{\text{Bohr}}, B(v) \, dv_{\text{Bohr}})$. Here, on the contrary, the physical Hilbert space is $L^2_S(\mathbb{R}_{\text{Bohr}}, \tilde{B}(v) \, dv_{\text{Bohr}})$.

This difference corresponds to different structures in the WDW theory. In [8], the physical Hilbert space in the corresponding WDW theory is $L^2_S(\mathbb{R}, B(v) \, dv)$, which is different from $L^2_S(\mathbb{R}, B(\mu) \, d\mu)$. [Note: $\tilde{B}(v) = \frac{1}{|v|^3/2}$ and $B(v) \to \tilde{B}(v)$ when $|v| \gg 1$.] Here, on the other hand, the physical Hilbert space is $L^2_S(\mathbb{R}, \tilde{B}(v) \, dv)$. [Note: $\tilde{B}(v)$ is defined such that $B(v) \, dv = B(\mu) \, d\mu$ and we have $B(v) \to \tilde{B}(v)$ when $|v| \gg 1$.] This difference can be understood as two different choices of factor ordering both in LQC and WDW theories. Both choices of factor ordering have their own advantages.

The approach used in this paper by introducing $\tilde{B}(v)$ (and $\tilde{B}(\vec{v})$ for the anisotropic case) is to insist the same WDW theory for both $\mu$-scheme (or say $\mu_o$-scheme for the isotropic case) and $\bar{\mu}$-scheme, even though the LQC theory is modified from $\mu$-scheme to $\bar{\mu}$-scheme. The advantage of this choice is two-fold. Firstly, the expression of the constraint equation is simpler. Secondly, since the WDW theory is unchanged, all we have to do in $\bar{\mu}$-scheme is changing variables from $\mu_I$ to $v_I$. Therefore, we can quite straightforwardly “translate” the results we obtained in Section VI and Section VII to those in $\bar{\mu}$-scheme as what we did in Section VIII C and Section VIII D. However, the drawback of this factor ordering is that the gravitational part of the Hamiltonian constraint $\hat{C}^{(\bar{\mu})}_{\text{grav}}$ is not self-adjoint in $H^S_{\text{grav}}$. On the contrary, the choice made in [8] insists $\hat{C}^{(\bar{\mu})}_{\text{grav}}$ to be self-adjoint in $H^S_{\text{grav}}$ and yields the “natural” factor ordering of the WDW theory in accordance with the use of Laplace-Beltrami operator in geometrodynamics (see [8] for details). □

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