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Loop quantization of vacuum Bianchi I cosmology

M. Martín-Benito,* G. A. Mena Marugán,+ and T. Pawlowski‡
Instituto de Estructura de la Materia, CSIC, Serrano 121, 28006 Madrid, Spain
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We analyze the loop quantization of the family of vacuum Bianchi I spacetimes, a gravitational system of which classical solutions describe homogeneous anisotropic cosmologies. We rigorously construct the operator that represents the Hamiltonian constraint, showing that the states of zero volume completely decouple from the rest of quantum states. This fact ensures that the classical cosmological singularity is resolved in the quantum theory. In addition, this allows us to adopt an equivalent quantum description in terms of a well-defined densitized Hamiltonian constraint. This latter constraint can be regarded in a certain sense as a difference evolution equation in an internal time provided by one of the triad components, which is polymerically quantized. Generically, this evolution equation is a relation between the projection of the quantum states in three different sections of constant internal time. Nevertheless, around the initial singularity the equation involves only the two closest sections with the same orientation of the triad. This has a double effect: on the one hand, physical states are determined just by the data on one section, on the other hand, the evolution defined in this way never crosses the singularity, without the need of any special boundary condition. Finally, we determine the inner product and the physical Hilbert space employing group averaging techniques, and we specify a complete algebra of Dirac observables. This completes the quantization program.

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I. INTRODUCTION

Loop quantum cosmology (LQC) [1] is nowadays an active field of research, devoted to the application of the ideas and mathematical methods of the full theory of loop quantum gravity (LQG) [2–4] to symmetry reduced cosmological models. This application is useful at least in two respects. On the one hand, it allows us to learn and gain experience about issues that are still open in full LQG. On the other hand, in many cases the symmetry reduced models already give us information about physical questions of interest. The first attempts to apply the techniques of LQG to symmetry reduced models can be found in Ref. [5]. More recently, some homogeneous and isotropic models have been quantized to completion in the LQC framework [6–13] along the revisited lines presented in Ref. [14]. In particular, these studies provide new results about the fate of the classical singularities. Namely, the cosmological singularities are resolved dynamically in these models, as they are replaced with quantum bounces.

In this paper we will discuss the loop quantization of a homogeneous but anisotropic model: the Bianchi I spacetimes *in vacuo*. Some preliminary analyses on the quantization of the Bianchi I model using Ashtekar variables were already developed in Refs. [15,16]. The merit for the first systematic attempts to construct the kinematical Hilbert space and introduce a Hamiltonian constraint for the model in a loop quantization framework must be granted to Bojowald [17]. However, apart from technical issues concerning the definition of the quantum operators (and the prescription adopted to incorporate the presence of a gap in the area spectrum of LQG), the analysis of Ref. [17] was not complete inasmuch as it did not provide the physical Hilbert space, nor an algebra of Dirac observables. The first work that attempted to complete the Dirac quantization program, adapting the techniques presented in Ref. [14] to quantize polymerically the gravitational degrees of freedom of the Bianchi I spacetimes, was done by Chiou [18]. In that case, nonetheless, the considered homogeneous model was not in a vacuum, because it included a massless scalar field. Here we will employ the same kind of techniques although we will use a slightly different quantization prescription [19], which seems more suitable to make manifest some relevant aspects of the LQC approach, keep under rigorous control the definition of the quantum Hamiltonian constraint, and complete the analysis of the physical states. In particular, an important feature of the quantization proposed here is that it immediately leads to the decoupling of the quantum states with zero volume [20], so that they can be removed from the theory. Employing this fact, we will show that physical states can be described equivalently as solutions to a densitized Hamiltonian constraint. We will prove that the operator that represents this constraint is a well-defined self-adjoint operator. Furthermore, we will explicitly construct the solutions to the constraint, find the physical inner product, and determine a complete set of observables.

Most of the homogenous models analyzed so far in LQC [6–13], and, in particular, the mentioned work of Ref. [18], contain matter in the form of a homogeneous massless

*merce.martin@iem.cfmac.csic.es
+mena@iem.cfmac.csic.es
‡tomasz@iem.cfmac.csic.es

scalar field. This field, quantized in a standard (Schrödinger-like) way serves as an internal time, providing a well-defined notion of evolution. Here, in the vacuum case, such a useful object is no longer available. Hence we will explore the problem of quantizing the variable that plays the role of internal time in a polymeric way, a fact that may affect the conventional concept of evolution. In our case, we will choose as internal time one of the triad components. This choice will provide us with a certain notion of evolution, as we will discuss in Sec. VII.

The classical vacuum Bianchi I spacetimes generically possess an initial cosmological singularity, to which we will allocate the origin of time. One of the main motivations of our analysis is to discuss what happens with this singularity in the loop quantum theory. We will see that, since the zero-volume states are totally decoupled, nontrivial physical states contain no contribution from them. In this sense the initial classical singularity is resolved and disappears from the quantum theory. Furthermore, in the presented quantization there exists no correlation between the sectors of opposite orientations of the triads. Therefore, the defined evolution does not connect sectors corresponding to different orientations of the variable identified as the internal time. As a consequence, the singularity is not crossed and no additional branch of the universe emerges on the opposite side of it. The provided notion of evolution is well defined without the need to impose any special boundary condition to deal with the two orientations of the triads.

The polymeric quantization of the system leads to a densitized Hamiltonian constraint that can be viewed as a discrete evolution equation on quantum states. This equation is a recurrence relation, which generically relates the projection of the state in three consecutive sections of constant internal time. However, when one reaches the origin in the quantization presented in this paper, it reduces to a relation on the two sections with the smallest possible values of the discrete time, in the sector of triad orientations under study. As a result, the physical states are in fact determined by their data on a single section. The vector space of these data can be provided with an inner product and one attains in this way the physical Hilbert space.

An additional, important motivation for the analysis of the loop quantization of Bianchi I *in vacuo* comes from the consideration of a (much richer) family of cosmological spacetimes that contain inhomogeneities, namely, the linearly polarized Gowdy model with T^3 topology [21]. This is an infinite dimensional model that provides a most suitable arena for the attempt to extend the analysis of homogenous LQC to inhomogeneous situations. The subfamily of homogeneous solutions within this model is just the classical vacuum Bianchi I spacetimes with T^3 topology. From this perspective, the loop quantization of Bianchi I *in vacuo* is a preliminary step in order to face the quantization of the Gowdy cosmologies.

Let us also comment that, during the writing of this manuscript, another work on the loop quantization of Bianchi I has appeared [22] which presents some similarities with our treatment. That work, carried out independently to ours, considers a simplified version of the quantization, where the corrections owing to the regularization of the inverse triad operator are not incorporated, and describes the time evolution using a massless scalar field, like in Ref. [18].

The main body of this paper is organized as follows. In Sec. II we construct the kinematical Hilbert space on which we define the elementary operators of the theory. The Hamiltonian constraint of the model is represented as a symmetric operator in Sec. III, where we also show the decoupling of the zero-volume states. Employing this decoupling, we densitize the Hamiltonian constraint in Sec. IV, arriving to an equivalent quantum description of the system. The form of the densitized constraint allows us to decompose it in terms of one-dimensional operators, which are then analyzed in detail in Sec. V. The solutions to the constraint and the corresponding physical Hilbert space is determined in Sec. VI. Finally, in Sec. VII we discuss the results of our quantization and conclude.

II. KINEMATICS

As a first step towards the loop quantization of the vacuum Bianchi I spacetimes, we describe the model in terms of Ashtekar variables [18,23]. In principle, the definition of these variables makes use of a finite sized cell and a fiducial triad. Adopting a diagonal gauge, it was shown in Ref. [23] that there is no physical dependence on the choice of fiducial triad if one defines the homogenous canonical variables for the model in a suitable way. For the sake of simplicity, we will then particularize the discussion to the choice of a diagonal Euclidean triad. The issue of the dependence on the coordinate cell of integration is more subtle [23]. Nonetheless, when the spatial sections of the Bianchi I cosmologies have a compact topology, there is a natural choice of coordinate cell. In fact, as we mentioned in the introduction, one of the motivations for our study is the potential application to the quantization of the homogeneous sector of the linearly polarized T^3-Gowdy model [21]. Consequently, we will specialize our analysis to a compact three-torus topology, adopting the corresponding natural cell for our treatment, namely, the T^3-cell with sides of coordinate length equal to 2π. In this way, one arrives at the following nontrivial components of the $SU(2)$ gravitational connection A_i^a and of the densitized triad E_a^i [24],

$$A_i^a = \frac{c^i}{2\pi}\,\delta_i^a, \qquad E_a^i = \frac{p_i}{4\pi^2}\,\delta_a^i, \tag{1}$$

so that $\{c^i, p_j\} = 8\pi G\gamma\delta_j^i$. Here $i, j = 1, 2$, or 3 are spatial indices, a is an internal $SU(2)$ index, G is the Newton constant, and γ is the Barbero-Immirzi parameter.

The spacetime metric written in terms of the variables p_i takes the form

$$ds^2 = -N^2dt^2 + \frac{|p_1p_2p_3|}{4\pi^2}\left[\sum_{i=1}^{3}\frac{(dx^i)^2}{p_i^2}\right], \tag{2}$$

where $\{dx^i\}$ is the fiducial co-triad, with $x^i \in S^1$, and N is the lapse function.

In LQC, one adapts the techniques of LQG to symmetry reduced systems in order to construct the kinematical Hilbert space [14,17,18]. The configuration variables are provided by holonomies along edges oriented in the fiducial directions, and the momentum variables by triad fluxes through fiducial rectangles orthogonal to those directions. The holonomy along an edge of oriented coordinate length $2\pi\mu_i$ in the direction i is

$$h_i^{\mu_i}(c^i) = e^{\mu_i c^i \tau_i}, \tag{3}$$

where τ_i are the $SU(2)$ generators proportional to the Pauli matrices, such that $[\tau_i, \tau_j] = \epsilon_{ijk}\tau^k$. The flux through the rectangle of coordinate area S^i orthogonal to the direction i turns out to be

$$E[S^i] = \frac{p_i}{4\pi^2}S^i. \tag{4}$$

The configuration algebra is obtained from the sums of products of matrix elements of the irreducible representations of the holonomies and is just the algebra of almost periodic functions of c^i [14,18]. This algebra is generated by the exponentials

$$\mathcal{N}_{\mu_i}(c^i) = e^{i\mu_i c^i/2}, \tag{5}$$

which, using the Dirac ket notation, will be represented by the states $|\mu_i\rangle$. The finite linear combinations of products of these functions provide the analog of the space of cylindrical functions in LQG, and we will call it Cyl_S. Thus, denoting $|\mu_1, \mu_2, \mu_3\rangle = \otimes_i|\mu_i\rangle$, we have

$$\mathrm{Cyl}_S = \mathrm{span}\{|\mu_1, \mu_2, \mu_3\rangle\}. \tag{6}$$

The kinematical Hilbert space $\mathcal{H}_{\mathrm{Kin}} = \otimes_i\mathcal{H}^i_{\mathrm{Kin}}$ is the completion of the space Cyl_S with respect to the discrete inner product $\langle\mu_i|\mu_i'\rangle = \delta_{\mu_i\mu_i'}$ for each direction [14,18]. The states $|\mu_i\rangle$ provide an orthonormal basis for $\mathcal{H}^i_{\mathrm{Kin}}$. They are eigenstates of the operator $\hat{p}_i$ associated with fluxes, while $\hat{\mathcal{N}}_{\mu_i'}$ simply shifts their label μ_i:

$$\hat{p}_i|\mu_i\rangle = 4\pi\gamma l_{\mathrm{Pl}}^2\mu_i|\mu_i\rangle, \tag{7}$$

$$\hat{\mathcal{N}}_{\mu_i'}|\mu_i\rangle = |\mu_i + \mu_i'\rangle. \tag{8}$$

Here, $l_{\mathrm{Pl}} = \sqrt{G\hbar}$ is the Planck length.

In LQG, the operator that represents the physical area has a discrete spectrum, with a minimum nonzero eigenvalue equal to $\Delta = 2\sqrt{3}\pi\gamma l_{\mathrm{Pl}}^2$. It has been argued that, when one takes into account this fact, a minimum coordinate length for the edge of the holonomies is introduced in LQC [8]. The exact form in which such a minimum coordinate length must be incorporated is still under discussion. At present, two prescriptions are considered in the literature [23,25]. Here we will adopt the prescription introduced in Ref. [18], usually called the $\bar{\mu}$ scheme. One of the advantages of this prescription is that (as we will see) the quantum analysis of the system can be carried out to completion, and not just in an effective, nonfundamental way. Besides, this will allow us to revisit some parts of the analysis presented in Ref. [18] which, to date, is the most complete discussion of the loop quantization of the Bianchi I model. In doing so, we will see that one can also learn some lessons about the quantization of other homogeneous systems like the isotropic ones. On the other hand, although the justification of this prescription from the viewpoint of the full theory of LQG is currently under investigation [26], it is important to note that there are no inconsistencies or nonphysical effects associated with it in cases with compact spatial topology like the one considered here, cases when a privileged coordinate cell exists [27].

According to this $\bar{\mu}$ scheme, the minimum coordinate length for each direction i is determined by the condition $\bar{\mu}_i^2|p_i| = \Delta$, from which we arrive at the operator relation

$$\frac{1}{\widehat{\bar{\mu}_i}} = \frac{\widehat{\sqrt{|p_i|}}}{\sqrt{\Delta}}. \tag{9}$$

Operators like $\widehat{\sqrt{|p_i|}}$ are defined in terms of $\hat{p}_i$ by means of the associated spectral decomposition. Acting on a state $|\mu_i\rangle$, we then get

$$\frac{1}{\widehat{\bar{\mu}_i}}|\mu_i\rangle = \frac{1}{\bar{\mu}_i(\mu_i)}|\mu_i\rangle, \qquad \bar{\mu}_i(\mu_i) = \sqrt{\frac{\sqrt{3}}{2|\mu_i|}}. \tag{10}$$

Since the value $\bar{\mu}_i$ is state-dependent, the associated operator $\hat{\mathcal{N}}_{\bar{\mu}_i}$ generates a state-dependent minimum shift. To write down its action, it is convenient to relabel the states by reparametrizing μ_i so that the minimum shift becomes uniform. This is achieved by introducing, for each direction, a label $v_i(\mu_i)$ which satisfies the equation

$$\bar{\mu}_i(\mu_i)\frac{\partial}{\partial\mu_i} = \frac{\partial}{\partial v_i}, \tag{11}$$

whose solution is

$$v_i(\mu_i) = \sqrt{\frac{2^3}{3^{5/2}}}\mathrm{sgn}(\mu_i)|\mu_i|^{3/2}. \tag{12}$$

With this relabeling, the basic operators have the following action in the domain Cyl_S:

$$\hat{p}_i|v_i\rangle = 3^{1/3}\Delta\,\mathrm{sgn}(v_i)|v_i|^{2/3}|v_i\rangle, \tag{13}$$

$$\hat{\mathcal{N}}_{\bar{\mu}_i}|v_i\rangle = |v_i + 1\rangle. \tag{14}$$

III. HAMILTONIAN CONSTRAINT

In the considered model, only one constraint remains to be imposed once the diagonal gauge has been chosen: the Hamiltonian constraint. In order to represent it as an operator, one first needs to express this constraint as a phase space function in terms of triads and holonomies, since there do not exist well-defined operators corresponding to the connection components c^i. This is done by the standard procedures of LQC, explained in detail in Ref. [18]. In brief, one defines the curvature components employing holonomies along edges of coordinate length $2\pi\bar{\mu}_i$ and regularizes the inverse of the determinant of the metric following Thiemann's procedure [2], i.e., expressing it via the Poisson bracket of holonomies with the volume function. Applying these procedures and setting the lapse $N = 1$, we arrive at the following form for the Hamiltonian constraint [18] (integrated over the chosen T^3-cell and still viewed as a classical function on phase space)

$$C_{\mathrm{BI}} = -\frac{2}{\gamma^2}\Big[\Lambda_1\Lambda_2\Big(\frac{1}{\sqrt{|p_3|}}\Big)_{\mathrm{reg}} + \Lambda_1\Lambda_3\Big(\frac{1}{\sqrt{|p_2|}}\Big)_{\mathrm{reg}} + \Lambda_2\Lambda_3\Big(\frac{1}{\sqrt{|p_1|}}\Big)_{\mathrm{reg}}\Big], \tag{15}$$

where

$$\Lambda_i = \frac{\sqrt{|p_i|}}{\bar{\mu}_i}\,\mathrm{sgn}(p_i)\sin(\bar{\mu}_i c^i), \tag{16}$$

and $(1/\sqrt{|p_i|})_{\mathrm{reg}}$ is the regularized expression for $1/\sqrt{|p_i|}$ obtained via Thiemann's method.

By the mentioned standard LQC procedures, this regularized phase space function is represented by the operator

$$\Big[\widehat{\frac{1}{\sqrt{|p_i|}}}\Big] = \frac{1}{4\pi\gamma l_{\mathrm{Pl}}^2} \times \frac{1}{\widehat{\bar{\mu}_i\,\mathrm{sgn}(p_i)}(\hat{\mathcal{N}}_{-\bar{\mu}_i}\widehat{\sqrt{|p_i|}}\hat{\mathcal{N}}_{\bar{\mu}_i} - \hat{\mathcal{N}}_{\bar{\mu}_i}\widehat{\sqrt{|p_i|}}\hat{\mathcal{N}}_{-\bar{\mu}_i})}, \tag{17}$$

where, for the $\bar{\mu}$ scheme that we have adopted, $\frac{1}{\bar{\mu}_i}$ and $\hat{\mathcal{N}}_{\bar{\mu}_i}$ are the operators defined in Eqs. (9) and (14), respectively. Note that there is no factor ordering ambiguity in the above formula, inasmuch as the operator in parenthesis commutes with all the others on the right-hand side of Eq. (17). Besides, it is easy to check that the states $|v_i\rangle$ are eigenstates of the introduced operator. Explicitly,

$$\Big[\widehat{\frac{1}{\sqrt{|p_i|}}}\Big]|v_i\rangle = b(v_i)|v_i\rangle,$$

$$b(v_i) = \frac{3^{5/6}}{2\sqrt{\Delta}}|v_i|^{1/3}||v_i + 1|^{1/3} - |v_i - 1|^{1/3}|. \tag{18}$$

In order to construct a symmetric operator $\hat{C}_{\mathrm{BI}}$ representing the Hamiltonian constraint (15), let us now consider the quantum counterpart of Λ_i. From Eq. (9), it follows that all the factors in Λ_i depend only on p_i except for $\sin(\bar{\mu}_i c^i)$. This latter term can be represented by the operator

$$\widehat{\sin(\bar{\mu}_i c^i)} = \frac{1}{2i}(\hat{\mathcal{N}}_{2\bar{\mu}_i} - \hat{\mathcal{N}}_{-2\bar{\mu}_i}), \tag{19}$$

which does not commute with $\hat{p}_i$. To obtain a symmetric operator for Λ_i, we then proceed as follows. Since the operator

$$\widehat{\sqrt{|p_i|}}\,\frac{1}{\widehat{\bar{\mu}_i = \frac{1}{\sqrt{\Delta}}\sqrt{|p_i|}}} \tag{20}$$

is non-negative, we can take its square root and adopt the symmetric factor ordering

$$\hat{\Lambda}_i = \frac{1}{2\sqrt{\Delta}}\widehat{\sqrt{|p_i|}}[\widehat{\sin(\bar{\mu}_i c^i)}\,\widehat{\mathrm{sgn}(p_i)} + \widehat{\mathrm{sgn}(p_i)}\,\widehat{\sin(\bar{\mu}_i c^i)}]\widehat{\sqrt{|p_i|}}. \tag{21}$$

Several comments are in order at this point. First, it is important to realize the presence of the factor $\mathrm{sgn}(p_i)$ in the expression of Λ_i, which was not properly taken into account in Ref. [18]. As a function on phase space, it does not commute with $\sin(\bar{\mu}_i c^i)$ under Poisson brackets, and hence their product as operators is not symmetric. Probably, its appearance had not been pointed out so far because, in the passage to the best studied case of (homogeneous and) isotropic LQC, a simplification occurs that makes its role less important. Up to a constant factor, the purely gravitational part of the Hamiltonian constraint for isotropic models can be obtained from Eq. (15) by identifying the three spatial directions [8,18]. In doing so, this gravitational part gets a factor of a squared sign that can be considered equal to the unity and ignored, instead of dealing with it as we have discussed for the anisotropic case. These two alternatives for the isotropic models can be understood as different choices of factor ordering. We have checked that a factor ordering like the one suggested here does not alter significantly the numerical results of Refs. [7,8] (in fact, for situations of physical interest, the difference is below the numerical errors). Nonetheless, even for the isotropic case our factor ordering may be more convenient in order to clarify certain conceptual and technical issues, like e.g. the decoupling of the zero-volume states or the properties of the solutions to the

constraint near the cosmological singularity, as we will see later on.

In addition, it is important to notice that the operator $\hat{\Lambda}_i$ annihilates the state $|v_i = 0\rangle$, which belongs to the kernel of $\hat{p}_i$. Furthermore, the range of $\hat{\Lambda}_i$ does not contain the alluded state, so that its orthogonal complement in $\mathcal{H}^i_{\rm Kin}$ is invariant under the action of $\hat{\Lambda}_i$. In particular, this ensures that the action of the operator $\widehat{\rm sgn}(p_i)$ present in $\hat{\Lambda}_i$ is well defined [28].

The factor ordering adopted in the quantum Hamiltonian constraint has some important advantages with respect to that proposed in Ref. [18]. First, the constraint is now a sum of products of symmetric operators, each defined on one of the Hilbert spaces $\mathcal{H}^i_{\rm Kin}$ associated with each direction. As we will see, this facilitates the determination of observables and makes the construction of physical solutions straightforward, thus allowing one to complete the quantization. Second, it is easy to check that the Hamiltonian constraint annihilates the proper subspace $\mathcal{H}^0_{\rm Kin}$ of states in the kernel of any of the operators $\hat{p}_i$. Such subspace is the completion of the subset of Cyl_S given by $\mathrm{Cyl}^0_S = \mathrm{span}\{|v_1, v_2, v_3\rangle; v_1 v_2 v_3 = 0\}$. Since $\hat{V} = \otimes_i \widehat{\sqrt{|p_i|}}$ is the volume operator, we will call $\mathcal{H}^0_{\rm Kin}$ the subspace of zero-volume states. Furthermore, the properties of the operator $\hat{\Lambda}_i$ commented above imply that the orthogonal complement of $\mathcal{H}^0_{\rm Kin}$ is invariant under the action of the constraint $\hat{C}_{\rm BI}$. Thus, the subspace of zero-volume states decouples from its complement and we can ignore it in the following, restricting our considerations exclusively to the subspace of nonzero-volume states. We will call this subspace $\tilde{\mathcal{H}}_{\rm Kin}$, whereas $\widetilde{\mathrm{Cyl}}_S$ will denote the corresponding linear span of tensor products of states $|v_i\rangle$ such that none of the v_i's vanishes.

As we will discuss in the next section, the decoupling of the zero-volume states allows one to describe the quantum system in a completely equivalent way in terms of a densitized version of the Hamiltonian constraint. Moreover, since nontrivial physical states get no contribution from zero-volume states, the classical initial singularity disappears from the quantum theory, already at the kinematical level. At least in this sense, the singularity is resolved quantum mechanically, in a way similar to that originally suggested by Bojowald [17] (see nonetheless [29]). We will consider this issue in more detail in the last section.

IV. DENSITIZED HAMILTONIAN CONSTRAINT

In order to solve the quantum constraint, it proves convenient to recast it in a densitized form which is easier to analyze. One should remember that physical states are states annihilated by the Hamiltonian constraint $\hat{C}_{\rm BI}$ and, in principle, they do not have to be normalizable in the kinematical Hilbert space $\tilde{\mathcal{H}}_{\rm Kin}$. More precisely, we expect these states to live in a larger space, namely, the algebraic dual $\widetilde{\mathrm{Cyl}}^*_S$ of the dense set $\widetilde{\mathrm{Cyl}}_S$. We will denote one such state by $(\psi|$.

In order to densitize the quantum Hamiltonian constraint in a rigorous manner, we have to invert the action of the operator

$$\widehat{\left[\frac{1}{V}\right]} = \otimes_i \widehat{\left[\frac{1}{\sqrt{|p_i|}}\right]} \tag{22}$$

which (via Thiemann's procedure) entered in the definition of our constraint. At this point, the observation that the zero-volume states decouple is essential, because the kernel of the operator (22) coincides precisely with that subspace. Thus, the inverse operator $\widehat{[1/V]}^{-1}$ is well defined once we have restricted ourselves to $\tilde{\mathcal{H}}_{\rm Kin}$. Note also that this densitization can be carried out exactly, without the need to simplify the theory by ignoring the quantum corrections coming from the regularized inverse volume operator (i.e., without replacing $\widehat{[1/V]}^{-1}$ by $\hat{V}$).

To reformulate the constraint in its densitized version, we introduce the following bijection in the dual $\widetilde{\mathrm{Cyl}}^*_S$

$$(\psi| \to (\psi| \widehat{\left[\frac{1}{V}\right]}^{1/2}. \tag{23}$$

The transformed physical states are now annihilated by the (adjoint of the) symmetric densitized Hamiltonian constraint $\hat{\mathcal{C}}_{\rm BI}$, defined as

$$\hat{\mathcal{C}}_{\rm BI} = \widehat{\left[\frac{1}{V}\right]}^{-1/2} \hat{C}_{\rm BI} \widehat{\left[\frac{1}{V}\right]}^{-1/2}. \tag{24}$$

Its explicit form is

$$\hat{\mathcal{C}}_{\rm BI} = -\frac{2}{\gamma^2}[\hat{\Theta}_1\hat{\Theta}_2 + \hat{\Theta}_1\hat{\Theta}_3 + \hat{\Theta}_2\hat{\Theta}_3], \tag{25}$$

where $\hat{\Theta}_i$ is the symmetric operator

$$\hat{\Theta}_i = \widehat{\left[\frac{1}{\sqrt{|p_i|}}\right]}^{-1/2} \hat{\Lambda}_i \widehat{\left[\frac{1}{\sqrt{|p_i|}}\right]}^{-1/2}. \tag{26}$$

This operator has the following action on the basis states $|v_i\rangle$:

$$\hat{\Theta}_i|v_i\rangle = -i\frac{\Delta}{2\sqrt{3}}[f_+(v_i)|v_i + 2\rangle - f_-(v_i)|v_i - 2\rangle], \tag{27}$$

where

$$f_\pm(v_i) = g(v_i \pm 2)s_\pm(v_i)g(v_i), \tag{28}$$

$$s_\pm(v_i) = \mathrm{sgn}(v_i \pm 2) + \mathrm{sgn}(v_i), \tag{29}$$

and

$$g(v_i) = \begin{cases} ||1+\frac{1}{v_i}|^{1/3} - |1-\frac{1}{v_i}|^{1/3}|^{-1/2} & \text{if } v_i \neq 0, \\ 0 & \text{if } v_i = 0. \end{cases} \quad (30)$$

V. ANALYSIS OF THE CONSTRAINT OPERATOR

One of the advantages of our quantization procedure is that, in order to study the properties of the constraint operator $\hat{C}_{\rm BI}$, we only need to analyze the operator $\hat{\Theta}_i$ on $\tilde{\mathcal{H}}^i_{\rm Kin}$. We carry out that analysis in this section.

A. Superselection

As we see in Eq. (27), $\hat{\Theta}_i$ is a difference operator with a step of two units in the label v_i. Given the definitions (28)–(30), the function $f_+(v_i)$ vanishes in the whole interval $v_i \in [-2, 0]$, while $f_-(v_i)$ is equal to zero for $v_i \in [0, 2]$. Owing to this remarkable property, which can be traced back to our treatment of the factor $\mathrm{sgn}(p_i)$ in the constraint, the operator $\hat{\Theta}_i$ does not relate states $|v_i\rangle$ with $v_i > 0$ to those with $v_i < 0$. Therefore, $\hat{\Theta}_i$ connects only states with labels v_i belonging to one of the semilattices

$$\mathcal{L}^{\pm}_{\varepsilon_i} = \{\pm(\varepsilon_i + 2k), k \in \mathbb{N}\}, \quad (31)$$

where

$$\mathbb{N} = \mathbb{N}^+ \cup \{0\}, \qquad \varepsilon_i \in (0, 2]. \quad (32)$$

Semilattices corresponding to different values of ε_i or to different signs are not connected by the action of $\hat{\Theta}_i$. In other words, the Hilbert space $\mathcal{H}^{\pm}_{\varepsilon_i}$, defined as the Cauchy completion of the set

$$\mathrm{Cyl}^{\pm}_{\varepsilon_i} = \mathrm{span}\{|v_i\rangle; v_i \in \mathcal{L}^{\pm}_{\varepsilon_i}\} \quad (33)$$

with respect to the discrete inner product, is invariant under the action of $\hat{\Theta}_i$. Note that the kinematical Hilbert space for each direction, which is not separable, can be decomposed into these separable Hilbert spaces:

$$\tilde{\mathcal{H}}^i_{\rm Kin} = \oplus_{\varepsilon_i}(\mathcal{H}^+_{\varepsilon_i} \oplus \mathcal{H}^-_{\varepsilon_i}). \quad (34)$$

Because of the absence of physically relevant operators that connect the different semilattices, the physical Hilbert space is then divided into superselection sectors. We can therefore restrict our study to any specific Hilbert space $\mathcal{H}^+_{\vec{\varepsilon}} = \otimes_i \mathcal{H}^+_{\varepsilon_i}$, with $\vec{\varepsilon} = (\varepsilon_1, \varepsilon_2, \varepsilon_3)$. Equivalently, we could construct the theory using e.g. the Hilbert space $\mathcal{H}^-_{\vec{\varepsilon}} = \otimes_i \mathcal{H}^-_{\varepsilon_i}$, since the constraint is symmetric under a flip of sign in the label v_i, owing to the identity

$$f_{\pm}(-v_i) = -f_{\mp}(v_i). \quad (35)$$

Finally, we would like to emphasize that the state $|v_i{=}0\rangle$ is not included in any of the superselection sectors, since it had been removed from the kinematical Hilbert space. The semilattices which one might expect to be connected with this state under the action of the constraint are those corresponding to $\varepsilon_i = 2$, but one can explicitly check that $\hat{\Theta}_i$ is indeed a completely well-defined operator on $\mathcal{H}^{\pm}_{\varepsilon_i}$ with domain $\mathrm{Cyl}^{\pm}_{\varepsilon_i}$. Nothing special occurs in the case $\varepsilon_i = 2$ in comparison with the other possible superselection sectors.

B. Spectral analysis

In order to determine the spectral properties of the operator $\hat{\Theta}_i$ it is helpful to first analyze its square. This squared operator is also important by itself as it represents (up to a multiplicative constant) the gravitational part of the densitized constraint in the isotropic case, where the elementary variables corresponding to the three different spatial directions are identified.

One can easily check that $\hat{\Theta}^2_i$ is a difference operator of constant step equal to four in the label v_i. Its action couples only those points v_i which lay on one of the semilattices

$${}^{(4)}\mathcal{L}^{\pm}_{\tilde{\varepsilon}_i} = \{\pm(\tilde{\varepsilon}_i + 4k), k \in \mathbb{N}\}, \qquad \tilde{\varepsilon}_i \in (0, 4]. \quad (36)$$

Thus, $\hat{\Theta}^2_i$ leaves invariant each of the Hilbert spaces ${}^{(4)}\mathcal{H}^{\pm}_{\tilde{\varepsilon}_i}$ obtained by the completion of

$${}^{(4)}\mathrm{Cyl}^{\pm}_{\tilde{\varepsilon}_i} = \mathrm{span}\{|v_i\rangle; v_i \in {}^{(4)}\mathcal{L}^{\pm}_{\tilde{\varepsilon}_i}\}. \quad (37)$$

If one now defines $\hat{\Theta}^2_i$ in ${}^{(4)}\mathcal{H}^+_{\tilde{\varepsilon}_i} \oplus {}^{(4)}\mathcal{H}^-_{4-\tilde{\varepsilon}_i}$ [with domain ${}^{(4)}\mathrm{Cyl}^+_{\tilde{\varepsilon}_i} \cup {}^{(4)}\mathrm{Cyl}^-_{4-\tilde{\varepsilon}_i}$], it is not difficult to check that its difference with respect to the operator $H'_{\rm APS}\Delta^2/(\pi G)$ defined in Ref. [9] [see Eq. (37) in that reference] is just a symmetric, trace class operator. For the particular case $\tilde{\varepsilon}_i = 4$, we can establish the same kind of comparison with $H'_{\rm APS}$ by starting with the Hilbert space ${}^{(4)}\mathcal{H}^+_4 \oplus {}^{(4)}\mathcal{H}^-_4$ and then including the state $|v_i = 0\rangle$, defining e.g. a vanishing action of $\hat{\Theta}^2_i$ on it.

Using the results obtained in Ref. [9] about the operator $H'_{\rm APS}$ and Kato's perturbation theory [30], it is straightforward to prove that $\hat{\Theta}^2_i$ is a positive, essentially self-adjoint operator whose essential spectrum and absolutely continuous spectrum are $[0, \infty)$ [31,32].

On the other hand, since $\hat{\Theta}^2_i$ leaves invariant ${}^{(4)}\mathcal{H}^{\pm}_{\tilde{\varepsilon}_i}$, its restriction to ${}^{(4)}\mathcal{H}^+_{\tilde{\varepsilon}_i} \oplus {}^{(4)}\mathcal{H}^-_{4-\tilde{\varepsilon}_i}$ (which has been analyzed above) commutes e.g. with the projection onto the subspace ${}^{(4)}\mathcal{H}^+_{\tilde{\varepsilon}_i}$. As a consequence, we conclude that $\hat{\Theta}^2_i$ on the Hilbert space ${}^{(4)}\mathcal{H}^+_{\tilde{\varepsilon}_i}$ [with domain ${}^{(4)}\mathrm{Cyl}^+_{\tilde{\varepsilon}_i}$] is essentially self-adjoint. Otherwise its deficiency index equation would have nontrivial solutions that would provide also valid solutions for the case in which the operator is defined on the larger Hilbert space ${}^{(4)}\mathcal{H}^+_{\tilde{\varepsilon}_i} \oplus {}^{(4)}\mathcal{H}^-_{4-\tilde{\varepsilon}_i}$, reaching a contradiction because we have already established that the operator is essentially self-adjoint in this latter case. Besides, for ${}^{(4)}\mathcal{H}^+_{\tilde{\varepsilon}_i}$, the essential spectrum and the absolutely continuous spectrum must still be $[0, \infty)$. One can

show it taking into account the symmetry of $\hat{\Theta}_i^2$ under a flip of sign in the label υ_i [see Eq. (35)] and accepting the independence of the spectrum on the value of $\tilde{\varepsilon}_i$. Moreover, numerical studies [33] indicate that the whole spectrum is just absolutely continuous. Indeed, the spectrum of $\hat{\Theta}_i^2$ [with domain ${}^{(4)}\mathrm{Cyl}_{\tilde{\varepsilon}_i}^+$] is nondegenerate and each of its eigenfunctions converges for large υ_i to a nonvanishing eigenfunction of the geometrodynamical (Wheeler-DeWitt) counterpart of the operator. This, together with the continuity of the spectrum in geometrodynamics, suffices to conclude that the discrete and singular spectra are empty [34].

In a manner similar to that explained above, one can also relate the solutions to the deficiency index equation of the operators $\hat{\Theta}_i^2$ and $\hat{\Theta}_i$ on $\mathcal{H}_{\varepsilon_i}^+ = {}^{(4)}\mathcal{H}_{\varepsilon_i}^+ \oplus {}^{(4)}\mathcal{H}_{2+\varepsilon_i}^+$ (both with domain $\mathrm{Cyl}_{\varepsilon_i}^+$). In this way, one can deduce that the specified operator $\hat{\Theta}_i$ is essentially self-adjoint. Therefore, we conclude that the constraint operator $\hat{\mathcal{C}}_{\mathrm{BI}}$, given in Eq. (25) and defined in the domain $\mathrm{Cyl}_{\tilde{\varepsilon}}^+ = \otimes_i \mathrm{Cyl}_{\varepsilon_i}^+$, is in fact essentially self-adjoint.

C. Generalized eigenstates

Taking into account the results of the previous subsection, we can obtain the spectral resolution of the identity associated with the operator $\hat{\Theta}_i$, e.g. on $\mathcal{H}_{\varepsilon_i}^+$, starting with those for the squared operator $\hat{\Theta}_i^2$ on ${}^{(4)}\mathcal{H}_{\varepsilon_i}^+$ and ${}^{(4)}\mathcal{H}_{2+\varepsilon_i}^+$. Remember that the spectrum of $\hat{\Theta}_i^2$ on any of these two Hilbert spaces is absolutely continuous and equal to the positive real line. For all ρ_i in the spectrum, we will call $|{}^{(4)}e_{\rho_i}^{\tilde{\varepsilon}_i})$ the corresponding generalized eigenstates normalized to the Dirac delta [35], where $\tilde{\varepsilon}_i = \varepsilon_i$ or $2 + \varepsilon_i$. Thus, on ${}^{(4)}\mathcal{H}_{\tilde{\varepsilon}_i}^+$ we have

$$\mathbb{I} = \int_{\mathbb{R}^+} d\rho_i |{}^{(4)}e_{\rho_i}^{\tilde{\varepsilon}_i})({}^{(4)}e_{\rho_i}^{\tilde{\varepsilon}_i}|. \tag{38}$$

In addition, we fix the global phase of these generalized eigenstates by choosing $({}^{(4)}e_{\rho_i}^{\tilde{\varepsilon}_i}|\upsilon_i\rangle$ to be a positive number for $\upsilon_i = \tilde{\varepsilon}_i$. In particular, this choice and the positivity of the operator $\hat{\Theta}_i^2$ ensure that $({}^{(4)}e_{\rho_i}^{\tilde{\varepsilon}_i}|\upsilon_i\rangle$ is real for all $\upsilon_i \in {}^{(4)}\mathcal{L}_{\tilde{\varepsilon}_i}^+$.

Renaming $\rho_i = \omega_i^2$ and combining the above resolutions of the identity for the Hilbert spaces ${}^{(4)}\mathcal{H}_{\varepsilon_i}^+$ and ${}^{(4)}\mathcal{H}_{2+\varepsilon_i}^+$, we obtain that, on their direct sum $\mathcal{H}_{\varepsilon_i}^+$,

$$\mathbb{I} = \int_{\mathbb{R}} d\omega_i |e_{\omega_i}^{\varepsilon_i})(e_{\omega_i}^{\varepsilon_i}|, \tag{39}$$

where, for $\omega_i \neq 0$,

$$\begin{aligned} |e_{+|\omega_i|}^{\varepsilon_i}) &= \sqrt{|\omega_i|}[|{}^{(4)}e_{\omega_i^2}^{\varepsilon_i}) - i|{}^{(4)}e_{\omega_i^2}^{2+\varepsilon_i})], \\ |e_{-|\omega_i|}^{\varepsilon_i}) &= \sqrt{|\omega_i|}[|{}^{(4)}e_{\omega_i^2}^{\varepsilon_i}) + i|{}^{(4)}e_{\omega_i^2}^{2+\varepsilon_i})]. \end{aligned} \tag{40}$$

For $\omega_i = 0$, we define

$$|e_0^{\varepsilon_i}) = |{}^{(4)}e_0^{\varepsilon_i}). \tag{41}$$

Recalling Eq. (27), one can check that the states $|e_{\omega_i}^{\varepsilon_i})$ defined above are generalized eigenstates of $\hat{\Theta}_i$ on $\mathcal{H}_{\varepsilon_i}^+$, with ω_i being the corresponding eigenvalue. Whence we find a real, absolutely continuous spectrum. Note also that the projections of $|e_{\omega_i}^{\varepsilon_i})$ on the Hilbert subspaces ${}^{(4)}\mathcal{H}_{\varepsilon_i}^+$ and ${}^{(4)}\mathcal{H}_{2+\varepsilon_i}^+$ (which are generalized eigenstates of the squared operator $\hat{\Theta}_i^2$ except for $\omega_i = 0$, when one of the projection vanishes) have a relative phase of $\pm\pi/2$. As a consequence, the phase of

$$e_{\omega_i}^{\varepsilon_i}(\upsilon_i) = \langle \upsilon_i | e_{\omega_i}^{\varepsilon_i}) \tag{42}$$

oscillates rapidly when υ_i varies in the semilattice $\mathcal{L}_{\varepsilon_i}^+$.

Furthermore, using Eq. (27), the eigenvalue equation associated with the operator $\hat{\Theta}_i$ on $\mathcal{H}_{\varepsilon_i}^+$ leads to the recurrence equation

$$\begin{aligned} e_{\omega_i}^{\varepsilon_i}(2n+2+\varepsilon_i) = {} & \frac{g(2n-2+\varepsilon_i)}{g(2n+2+\varepsilon_i)} e_{\omega_i}^{\varepsilon_i}(2n-2+\varepsilon_i) \\ & - i\frac{\sqrt{3}\omega_i}{\Delta} \frac{e_{\omega_i}^{\varepsilon_i}(2n+\varepsilon_i)}{g(2n+2+\varepsilon_i)g(2n+\varepsilon_i)} \end{aligned} \tag{43}$$

$\forall\ n \in \mathbb{N}^+$, which involves three distinct values of υ_i, as it corresponds to a second-order difference equation. However, for $n = 0$ we get a relation between the two first coefficients of the generalized eigenstates,

$$e_{\omega_i}^{\varepsilon_i}(2+\varepsilon_i) = -i\frac{\sqrt{3}\omega_i}{\Delta} \frac{e_{\omega_i}^{\varepsilon_i}(\varepsilon_i)}{g(2+\varepsilon_i)g(\varepsilon_i)}. \tag{44}$$

Therefore the solutions to the eigenvalue problem are totally determined by a simple piece of initial data, namely, the projection of the generalized eigenstate for the minimum allowed value of υ_i, $e_{\omega_i}^i(\varepsilon_i)$. Actually, a careful calculation shows that, $\forall\ n \in \mathbb{N}^+$,

$$\begin{aligned} e_{\omega_i}^{\varepsilon_i}(2n+\varepsilon_i) = {} & \sum_{O(n)} \Bigg[\prod_{\{r_p\}} \frac{g(2r_p+\varepsilon_i)}{g(2r_p+4+\varepsilon_i)} \Bigg] \\ & \times \Bigg[\prod_{\{s_q\}} \frac{-i\sqrt{3}\omega_i}{\Delta g(2s_q+2+\varepsilon_i)g(2s_q+\varepsilon_i)} \Bigg] \\ & \times e_{\omega_i}^{\varepsilon_i}(\varepsilon_i). \end{aligned} \tag{45}$$

Here, $O(n)$ denotes the set of all possible ways to move from 0 to n by jumps of one or two steps. For each element in $O(n)$, $\{r_p\}$ is the subset of integers followed by a jump of two steps, whereas $\{s_q\}$ is the subset of integers followed by a jump of only one step.

VI. THE PHYSICAL HILBERT SPACE

Once we have a good knowledge of the properties of the constraint operator, we turn to the issue of determining the physical Hilbert space in order to complete the quantization. Let $\mathcal{U}$ be the domain of the self-adjoint extension of the constraint operator $\hat{\mathcal{C}}_{\rm BI}$ on the superselection sector $\mathcal{H}^{+}_{\vec{\varepsilon}}$. Starting from the dense subset $\mathcal{U}$, we can obtain the physical Hilbert space, $\mathcal{H}^{\rm Phy}_{\vec{\varepsilon}}$, by applying the group averaging procedure [36,37]. Namely, given an element $|\phi\rangle$ in $\mathcal{U}$ [with corresponding wave function $\phi(\vec{v})$ in the $\vec{v}$ representation, where $\vec{v} = (v_1, v_2, v_3)$], one can "project" it onto $\mathcal{H}^{\rm Phy}_{\vec{\varepsilon}}$ via an average over the group generated by the constraint $\hat{\mathcal{C}}_{\rm BI}$:

$$\Phi(\vec{v}) = [\mathcal{P}\phi](\vec{v}) = \int_{\mathbb{R}} dt\, e^{it(\gamma^2/2)\hat{\mathcal{C}}_{\rm BI}}\phi(\vec{v}). \tag{46}$$

Employing the spectral decomposition associated with the operators $\hat{\Theta}_i$ for the three spatial directions, we can express the wave function $\phi(\vec{v})$ in terms of the eigenfunctions $e^{\varepsilon_i}_{\omega_i}(v_i)$ introduced in Eq. (42)

$$\phi(\vec{v}) = \int_{\mathbb{R}^3} d\vec{\omega}\, \bar{\phi}(\vec{\omega}) e^{\varepsilon_1}_{\omega_1}(v_1) e^{\varepsilon_2}_{\omega_2}(v_2) e^{\varepsilon_3}_{\omega_3}(v_3), \tag{47}$$

where $\vec{\omega} = (\omega_1, \omega_2, \omega_3)$, $\bar{\phi} \in L^2(\mathbb{R}^3, d\vec{\omega})$, and $v_i \in \mathcal{L}^{+}_{\varepsilon_i}$. Substituting this decomposition into Eq. (46), we then get

$$\Phi(\vec{v}) = \int_{\mathbb{R}^3} d\vec{\omega}\, \delta(\omega_1\omega_2 + \omega_1\omega_3 + \omega_2\omega_3) \times \bar{\phi}(\vec{\omega}) e^{\varepsilon_1}_{\omega_1}(v_1) e^{\varepsilon_2}_{\omega_2}(v_2) e^{\varepsilon_3}_{\omega_3}(v_3). \tag{48}$$

We immediately conclude from this expression that only products of eigenstates $|e^{\varepsilon_i}_{\omega_i}\rangle$ with $\sum_i (1/\omega_i) = 0$ will contribute to $\mathcal{H}^{\rm Phy}_{\vec{\varepsilon}}$. It is then useful to consider one of the ω_i's as a function of the others. Owing to the symmetry of the system under the interchange of the three directions, the particular choice of ω_i that one makes is just a matter of convention. Here we select ω_1. From now on, we define it as follows:

$$\omega_1(\omega_2, \omega_3) = -\frac{\omega_2\omega_3}{\omega_2 + \omega_3}. \tag{49}$$

With this choice, the wave function that represents the "projection" of the kinematical state $|\phi\rangle$ onto the physical Hilbert space takes the form

$$\Phi(\vec{v}) = \int_{\mathbb{R}^2} \frac{d\omega_2 d\omega_3}{|\omega_2 + \omega_3|} \Phi(\omega_2, \omega_3) e^{\varepsilon_1}_{\omega_1(\omega_2,\omega_3)}(v_1) \times e^{\varepsilon_2}_{\omega_2}(v_2) e^{\varepsilon_3}_{\omega_3}(v_3), \tag{50}$$

where $\Phi(\omega_2, \omega_3) = \bar{\phi}[\omega_1(\omega_2, \omega_3), \omega_2, \omega_3]$. We remember that the eigenfunctions $e^{\varepsilon_i}_{\omega_i}(v_i)$ that appear in the above expression are given (up to a normalization factor) by Eq. (45).

Employing this result and the delta-normalization of the generalized eigenstates of $\hat{\Theta}_i$, one can compute the physical inner product between two states $|\Phi_1\rangle$ and $|\Phi_2\rangle$

$$\langle\Phi_1|\Phi_2\rangle_{\rm Phy} = \langle\mathcal{P}\phi_1|\phi_2\rangle_{\rm Kin} = \int_{\mathbb{R}^2} \frac{d\omega_2 d\omega_3}{|\omega_2 + \omega_3|} \Phi_1^*(\omega_2, \omega_3)\Phi_2(\omega_2, \omega_3). \tag{51}$$

We have introduced the subindices "Phy" and "Kin" to distinguish between the inner products of the physical and the kinematical Hilbert spaces, and the symbol $*$ denotes complex conjugation. Therefore, the physical Hilbert space of the considered system is the space

$$\mathcal{H}^{\rm Phy}_{\vec{\varepsilon}} = L^2\left(\mathbb{R}^2, \frac{d\omega_2 d\omega_3}{|\omega_2 + \omega_3|}\right) \tag{52}$$

of square integrable functions on $\mathbb{R}^2$ with integration measure $d\omega_2 d\omega_3/|\omega_2 + \omega_3|$.

An alternative way to arrive at the physical Hilbert space is to find the space of solutions to the constraint and a complete set of (real) observables, imposing then the condition that these observables be self-adjoint in order to determine a Hilbert structure on the space of solutions. Once we know the spectral resolution of the identity associated with the operators $\hat{\Theta}_i$, it is straightforward to solve the constraint by adopting a formal expansion of the states in terms of the generalized eigenstates $|e^{\varepsilon_i}_{\omega_i}\rangle$, since $\hat{\mathcal{C}}_{\rm BI}$ has a diagonal action with this decomposition. Indeed, if we represent the candidate state by a wave function $\phi'(\omega_1, \omega_2, \omega_3)$, $\hat{\mathcal{C}}_{\rm BI}$ becomes just a polynomial constraint on ω_i. The physical solutions are described by functions of the form $\Phi'(\omega_2, \omega_3) = \phi'[\omega_1(\omega_2, \omega_3), \omega_2, \omega_3]$, where $\omega_1(\omega_2, \omega_3)$ is given by Eq. (49). A complete set of observables is provided e.g. by the operators $\hat{\Theta}_2$ and $\hat{\Theta}_3$, that multiply the wave function $\Phi'(\omega_2, \omega_3)$ by ω_2 and ω_3, respectively, and by the derivative operators $-i\partial_{\omega_2}$ and $-i\partial_{\omega_3}$. Demanding that they be self-adjoint, we arrive at the physical Hilbert space $L^2(\mathbb{R}^2, d\omega_2 d\omega_3)$. Under multiplication of the wave function by the factor $\sqrt{|\omega_2 + \omega_3|}$, one obtains in fact a unitarily equivalent representation of the algebra of observables on the Hilbert space given in Eq. (52).

VII. CONCLUSIONS AND DISCUSSION

In this work, we have presented a complete loop quantization of the family of homogeneous Bianchi I cosmologies *in vacuo*. We have described the quantum system in terms of a well-defined densitized Hamiltonian constraint, represented it by a(n essentially) self-adjoint operator, found the general form of its solutions, and determined the corresponding Hilbert space of physical states.

A nice property of the quantization that we have put forward, including the chosen factor ordering, is that the

quantum Hamiltonian constraint adopts the form of a sum of products of symmetric operators for each of the spatial directions. Under the densitization of the constraint, this allows one to reduce the analysis of self-adjointness and the spectral analysis just to the consideration of operators for one-dimensional systems (those describing independently each of the spatial directions).

Furthermore, our quantum Hamiltonian constraint annihilates the kernel of the volume operator and leaves invariant its orthogonal complement. As a consequence, the subspace of zero-volume states gets decoupled and one can ignore it in the study of the nontrivial physical states. This fact is essential to attain an equivalent formulation of the quantum system in terms of a densitized Hamiltonian constraint. This densitized constraint retains all the information about the quantum behavior of the model; in particular, it is not necessary to introduce simplifications that disregard the regularization of the inverse triad operators in LQC.

As it is common in polymeric quantizations, the physical Hilbert space is superselected. Physical states have support in semilattices that have a basic step of two units in the labels v_i. This differs from other previous analysis in LQC where the constructed superselection sectors correspond to entire lattices, with points distributed over the whole real line instead of over a semiaxis [6–14,17,18,22]. As we have seen in Sec. V, this facilitates the spectral analysis of the relevant difference operators and removes remnant global symmetries of the system, namely, those under reversal of the triad orientations (which now simply relate different superselection sectors). In addition, and related with these issues, all superselection sectors have essentially the same treatment in our quantization. Nothing special happens for the semilattices formed by even integers, which are those that the difference operators would connect with the origin had the zero-volume states not been decoupled.

As we have commented, the factor ordering that we have adopted reduces the functional analysis of the densitized constraint operator to that of the simple operator $\hat{\Theta}_i$. In addition, for the three possible directions i, these operators are immediately identified as Dirac observables. It is worth commenting on some of their properties in more detail. We have seen that $\hat{\Theta}_i$ behaves as a second-order difference operator in many aspects. Nonetheless, we know that it represents the classical variable $c^i p_i$, which would become a first-order differential operator in a standard canonical quantization of the Wheeler-DeWitt type. Therefore, one would expect that, if the results of the Wheeler-DeWitt approach are to be recovered in a certain regime from the loop quantization, the generalized eigenstates have to be determined from data on a single section of constant v_i. Remarkably, this is indeed the case.

This issue had not been pinpointed until now because in the homogeneous and isotropic models a subtle coincidence occurs. In that case, the gravitational part of the constraint is given by an operator like $\hat{\Theta}_i^2$. Such an operator, which represents the classical variable $(c^i p_i)^2$, behaves in fact as a second-order one in the Wheeler-DeWitt quantization.

Another difference with respect to previous analyses in LQC like those presented in Refs. [6–14,18,22] is that we have not introduced any matter content (and specifically no scalar field) as internal time. The variable identified with the internal time in our model is one of the triad components, which are quantized polymerically. Actually, the three diagonal triad components have an equivalent role because the model is symmetric under the interchange of spatial directions. We have selected the direction $i = 1$ to make the discussion explicit, but the choice is just a question of convention. Since the eigenstates of $\hat{\Theta}_1$ are determined by their initial data at $v_1 = \varepsilon_1$, the physical states get also fixed by data on this initial slice. Furthermore, the nondegeneracy of the spectrum of $\hat{\Theta}_1$ implies that the wave function at any v_1-constant slice determines the entire solution up to corrections of vanishing physical norm. Also the physical inner product can be rewritten in terms of data on that single section [38]. One can then admit the viewpoint that physical states evolve from this initial slice to any other slice, in such a way that they solve the densitized Hamiltonian constraint. As a consequence of the loop quantization adopted for the internal time, this concept of evolution differs from the usual one and, in particular, does not allow one to reach unitarity in a straightforward, standard way [33]. One should be aware that the notion of evolution used here refers only to the fact that there is a deterministic relation between data on two slices of constant internal time, and thus its meaning is certainly limited. Also, a preliminary analysis of the eigenfuctions shows that the evolution parameter (internal time) is not monotonic in the cosmic time, which makes the extraction of relevant physical data nontrivial.

On the other hand, the decoupling of the zero-volume states ensures that nontrivial physical states have no contribution from the slice where the curvature singularity is located in the classical theory. Physical states are well defined everywhere and, in this respect, the singularity is resolved quantum mechanically. This conclusion reinforces previous results about singularity resolution in LQC. It is worth emphasizing that this conclusion is independent of our choice of internal time. Furthermore, since the wave functions of the physical states (in the v_1 representation) have support just in semilattices, the evolution does not connect them with other branches of the universe, corresponding to a different orientation of the triads. The singularity is never crossed in the evolution. Let us also notice that this result is achieved without appealing to any kind of boundary conditions that might restrict the initial data for the physical states. As far as one understands the statement in this sense, one can say that physical states ''arise from

nothing'' in the initial slice $v_1 = \varepsilon_1$, attaining a no-boundary description.

Apart from the points addressed in this work about the loop quantization of the vacuum Bianchi I model, there are other interesting issues that we plan to explore in a future research [33]. This includes a detailed comparison with the Wheeler-DeWitt theory, the discussion of the concept of evolution, and the fate of unitarity in the model. We also want to carry out a numerical study of the physical states, analyzing, in particular, the occurrence of quantum bounces.

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