Physical evolution in loop quantum cosmology: The example of the vacuum Bianchi I modelMercedes Martín-Benito,^{*} Guillermo A. Mena Marugán,[†] and Tomasz Pawłowski[‡]*Instituto de Estructura de la Materia, CSIC, Serrano 121, 28006 Madrid, Spain*

(Received 22 June 2009; published 27 October 2009)

We use the vacuum Bianchi I model as an example to investigate the concept of physical evolution in loop quantum cosmology (LQC) in the absence of the massless scalar field which has been used so far in the literature as an internal time. In order to retrieve the system dynamics when no such a suitable clock field is present, we explore different constructions of families of unitarily related partial observables. These observables are parametrized, respectively, by: (i) one of the components of the densitized triad, and (ii) its conjugate momentum; each of them playing the role of an evolution parameter. Exploiting the properties of the considered example, we investigate in detail the domains of applicability of each construction. In both cases the observables possess a neat physical interpretation only in an approximate sense. However, whereas in case (i) such interpretation is reasonably accurate only for a portion of the evolution of the universe, in case (ii) it remains so during all the evolution (at least in the physically interesting cases). The constructed families of observables are next used to describe the evolution of the Bianchi I universe. The performed analysis confirms the robustness of the bounces, also in absence of matter fields, as well as the preservation of the semiclassicality through them. The concept of evolution studied here and the presented construction of observables are applicable to a wide class of models in LQC, including quantizations of the Bianchi I model obtained with other prescriptions for the improved dynamics.

DOI: 10.1103/PhysRevD.80.084038

PACS numbers: 04.60.Pp, 04.60.Kz, 98.80.Qc

I. INTRODUCTION

Loop quantum cosmology (LQC) [1] is an area of physics which deals with the quantization of symmetry reduced gravitational systems by adopting similar methods to those employed in loop quantum gravity [2].

Not surprisingly, the kinematical structure underlying LQC was rigorously established for the first time for the simplest of all the cosmological models, namely, those describing a homogeneous, isotropic, and spatially flat geometry [3]. The analysis of the dynamics of such a kind of geometry in the presence of a massless and minimally coupled scalar field has shown that the big bang singularity is resolved dynamically and is replaced by a quantum bounce [4,5]. LQC has been further extended, with diverse levels of rigor, to other similar models with different topology [6] or nonvanishing cosmological constant [7], and furthermore to more general settings such as anisotropic systems [8–10], or even to inhomogeneous situations [11]. The robustness of the singularity resolution features has been confirmed within an exactly solvable version of LQC [12–14], and the mathematical foundations of its elements have been discussed [15,16]. In addition to the studies of the genuine quantum theory, there exists an extensive amount of work at the level of the effective classical dynamics [17,18], which provides important insights into the properties of the quantum geometry in cosmological scenarios [19,20].

So far, all the analyses of the dynamics carried out in the genuine quantum theory have employed partial observables parametrized by an emergent time. In most of the models considered in the literature [4–8,10,12,14], the role of time was played by a massless scalar field, which (unlike the geometry degrees of freedom) was quantized adopting a standard Schroedinger-like representation. However, in many cases (vacuum homogeneous universes, black hole interiors) such possibility is not at hand. In this article, we overcome this difficulty by constructing and studying the properties of various families of unitarily related observables parametrized by the geometry degrees of freedom. As an appropriate test bed for our analysis, we study a model of a vacuum homogeneous universe of the Bianchi I type.

The Bianchi I system itself has been extensively analyzed in the literature. The quantization of this model using Ashtekar variables was already discussed in Refs. [21,22]. The loop quantization was first investigated in Ref. [23]. After that preliminary analysis of the kinematics, an attempt to complete the loop quantization of the model was made in Ref. [8], and the corresponding effective dynamics was studied in Ref. [24] (see also [25]). There, however, a homogeneous massless scalar field was coupled as matter content and identified as an internal time. The inclusion of a homogeneous magnetic field was also considered in Ref. [26].

Recently, the system *in vacuo* has been thoroughly quantized [9]. In that work, the studies were restricted to the model with the compact three-torus (T^3) topology, in order to provide a basis for further studies of a much more general system, namely, the inhomogeneous Gowdy T^3

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model with linear polarization [11]. In Ref. [9] both the physical Hilbert space and a complete algebra of observables were constructed; nonetheless the dynamics of the system was not investigated.

Let us comment that the extension of a quantization prescription known as improved dynamics from the isotropic to the anisotropic setting in homogenous LQC has given rise to the proposal of two concurrent prescriptions for Bianchi I. In this article, following Ref. [9], we use the prescription proposed in Ref. [8]. For noncompact models and just in the form presented in that paper, that prescription is not invariant under certain transformations [27], but for compact models, including the one considered in Ref. [9], the prescription is free from this drawback. The desired invariance is recovered in noncompact situations with an alternative prescription, which was recently developed and motivated in Ref. [10] appealing to the hypothesized relationship between the degrees of freedom of LQC and full LQG. For our discussion, nonetheless, the following reasons explain our use of the former of these prescriptions. (a) The goal of our work is a methodological development of a formalism of unitary evolution, defining it in a precise manner without introducing an additional matter field as a clock. For that purpose, the model of Ref. [9] is a better candidate, as the structure of the Hilbert space and the properties of the states are known in detail and have been presented in the literature, something which is necessary to establish the link between physical intuition and the exact mathematical implementation of our method. (b) The specific properties of the model of Ref. [9] allow to study the limitations of applicability of some of the constructed methods (see, in particular, Fig. 3 and the related discussion in Sec. V E), limitations which would have been missed had one used the model of Ref. [10]. (c) Our construction, although applied here to a concrete model, is intended to be reasonably universal. In particular, it is almost directly applicable to other possible prescriptions for the quantization of the Bianchi I model, including that of Ref. [10] (see the discussion in Sec. VII).

Employing the knowledge accumulated in previous works about the properties of the selected model, and the explicit and complete quantization chosen for it, we will analyze here two possible constructions of families of unitarily related observables, which are, respectively, parametrized by: (i) a coefficient of the densitized triad, and (ii) the variable conjugate to it. For the sake of clarity in the presentation, as well as for comparing the predictions of geometrodynamics and LQC, we will apply the construction to both the LQC version of the model and its Wheeler-DeWitt (WDW) counterpart. We will see that, whereas in a WDW-type quantization our construction with respect to both of the specified parameters provides observables with a precise physical interpretation, in the loop quantization scheme this property is achieved only in an approximate

sense. Furthermore, the accuracy of the interpretation depends only on properties of the state in case (ii), while for (i) the dependence is also on the evolution epoch.

The paper is organized as follows. Sec. II is a review of the LQC quantization of Ref. [9]. In Sec. III we perform the WDW quantization of the model and develop an interpretation for the evolution of observables for the two considered choices of internal time. In Sec. IV we show that the LQC states converge in a certain limit to a combination of WDW states. The evolution picture in the LQC theory is analyzed in Sec. V and VI for the choices of internal time (i) and (ii), respectively. In Sec. VII we discuss the main results of this work. Besides, two appendices are added. One of them extends the discussion on the WDW regime to take into account the union of different sectors. Finally, a brief description of the effective classical dynamics, associated with the genuine LQC dynamics, is given in Appendix B.

II. THE FRAMEWORK

In this section we briefly review the basic features of the polymerically quantized vacuum Bianchi I model. It is a summary of the main results obtained in Ref. [9], which the reader can consult for further details.

A. Classical theory

The Bianchi I model represents spatially flat and homogeneous spacetimes. We will consider the case of a compact topology: that of a three-torus. The spacetime metric can be written in the form [24]

$$ds^2 = -N^2 dt^2 + \frac{|p_1 p_2 p_3|}{4\pi^2} \sum_{i=1}^3 \frac{(dx^i)^2}{p_i^2}, \quad (2.1)$$

where $\{dx^i\}$ is the fiducial cotriad, N is the lapse function, and $p_i/(4\pi^2)$ are the nontrivial components of the densitized triad in a diagonal gauge. The corresponding components of the Ashtekar connection are $c^i/(2\pi)$, such that $\{c^i, p_j\} = 8\pi G \gamma \delta_j^i$. Here G is the Newton constant and γ is the Immirzi parameter (that we assume positive for simplicity). Owing to homogeneity, the only constraint present in the model is the Hamiltonian one, given by [24]

$$C_{\text{BI}} = -\frac{2}{\gamma^2} \frac{c^1 p_1 c^2 p_2 + c^1 p_1 c^3 p_3 + c^2 p_2 c^3 p_3}{V} = 0, \quad (2.2)$$

where $V = \sqrt{|p_1 p_2 p_3|}$ is the spacetime volume. Classically, any of the triad coefficients p_i is a monotonous function of the time coordinate t [24]. Moreover, the spacetime presents a curvature singularity at initial time $t = 0$, at which the universe stretches as an infinitely long line.

B. Loop quantum cosmology kinematics

In LQC the basic configuration variables are holonomies of connections. The holonomy along an edge of oriented coordinate length $2\pi\mu_i$ in the direction i is defined as $h_i^{\mu_i}(c^i) = e^{\mu_i c^i \tau_i}$, where τ_i are the $SU(2)$ generators proportional to the Pauli matrices, such that $[\tau_i, \tau_j] = \epsilon_{ijk} \tau^k$. The configuration algebra Cyl_S is the algebra of almost periodic functions of c^i , which is generated by the matrix elements of the holonomies $\mathcal{N}_{\mu_i}(c^i) = e^{(i/2)\mu_i c^i}$. In the momentum representation, the states defined by these matrix elements are denoted by $|\mu_i\rangle$. The completion of the algebra Cyl_S with respect to the discrete inner product $\langle \mu_i | \mu'_i \rangle = \delta_{\mu_i \mu'_i}$ for each fiducial direction provides the kinematical Hilbert space $\mathcal{H}_{\text{Kin}} = \otimes_i \mathcal{H}_{\text{Kin}}^i$. The elementary operators are the operators $\hat{p}_i$ associated with fluxes, which are diagonal on the basis states $|\mu_i\rangle$ of $\mathcal{H}_{\text{Kin}}^i$, and $\hat{\mathcal{N}}_{\mu'_i}$, whose action shifts the label μ_i of the considered basis by μ'_i .

In order to express C_{BI} in terms of holonomies, instead of connections components, one introduces the curvature tensor associated with the Ashtekar connection and defines it as in gauge lattice theories. With this aim, one considers a loop of holonomies and shrinks its area to its minimum value, which is nonzero owing to the discreteness of the area spectrum in LQG. To determine the minimum $2\pi\bar{\mu}_i$ for the coordinated length of the holonomy we assume (as in Ref. [8]) square loops of fiducial area $4\pi^2\bar{\mu}_i^2$ with minimum physical area equal to $\Delta = 2\sqrt{3}\pi\gamma l_{\text{Pl}}^2$, with $l_{\text{Pl}} = \sqrt{G\hbar}$ being the Planck length. This implies that $\bar{\mu}_i^2 |p_i| = \Delta$ in the sense of operators [28]. On the other hand, one appeals to the so-called ‘‘Thiemann’s trick’’ to define a well-defined inverse volume operator $[1/\widehat{V}]$. As a final result one obtains a quantum Hamiltonian constraint $\hat{C}_{\text{BI}}$ expressed in terms of our basic operators and which is well-defined in the domain Cyl_S [8,9].

Owing to the relation $\bar{\mu}_i^2 |p_i| = \Delta$, the shift produced by the operator $\hat{\mathcal{N}}_{\pm\bar{\mu}_i}$ on the basis states $|\mu_i\rangle$ is not constant. One can nevertheless relabel these states with an affine parameter

$$v_i(\mu_i) = 2^{3/2} 3^{-5/4} \text{sgn}(\mu_i) |\mu_i|^{3/2}, \quad (2.3)$$

to make the shift uniform [8,9]. The action of the basic operators in the relabeled states is $\hat{\mathcal{N}}_{\pm\bar{\mu}_i} |v_i\rangle = |v_i \pm 1\rangle$ and $\hat{p}_i |v_i\rangle = 3^{1/3} \Delta \text{sgn}(v_i) |v_i|^{2/3} |v_i\rangle$.

We have symmetrized the resulting Hamiltonian constraint $\hat{C}_{\text{BI}}$ in such a way that it annihilates the subspace spanned by the ‘‘zero-volume’’ states, i.e. the states $\otimes_i |v_i\rangle$ with any v_i equal to zero, and leaves invariant its orthogonal complement. For the nontrivial solutions to the constraint, we can thus restrict our study to that complement. Owing to this restriction the singularity is resolved at the kinematical level [9].

It is convenient to densitize the Hamiltonian constraint to find its solutions. The densitized Hamiltonian constraint is given by the operator

$$\hat{C}_{\text{BI}} = \left[\frac{1}{\widehat{V}} \right]^{-1/2} \hat{C}_{\text{BI}} \left[\frac{1}{\widehat{V}} \right]^{-1/2}, \quad (2.4)$$

which is well-defined in the considered domain (linear span of tensor products of states $|v_i\rangle$ such that none of the v_i ’s vanishes). The bijection $(\tilde{\psi} | = (\psi | [1/\widehat{V}]^{1/2}$ in the dual of that domain relates the nontrivial solutions $(\psi |$ of $\hat{C}_{\text{BI}}$ to the solutions $(\tilde{\psi} |$ of its densitized version $\hat{C}_{\text{BI}}$. This operator turns out to be given by

$$\hat{C}_{\text{BI}} = -\frac{2}{\gamma^2} [\hat{\Theta}_1 \hat{\Theta}_2 + \hat{\Theta}_1 \hat{\Theta}_3 + \hat{\Theta}_2 \hat{\Theta}_3], \quad (2.5)$$

where the operator $\hat{\Theta}_i$ is symmetric in the domain spanned by the basis states $|v_i\rangle$ ($v_i \neq 0$). Its action is:

$$\hat{\Theta}_i |v_i\rangle = -i \frac{\Delta}{2\sqrt{3}} [f_+(v_i) |v_i + 2\rangle - f_-(v_i) |v_i - 2\rangle], \quad (2.6)$$

where

$$f_{\pm}(v_i) = g(v_i \pm 2) s_{\pm}(v_i) g(v_i), \quad (2.7)$$

$$s_{\pm}(v_i) = \text{sgn}(v_i \pm 2) + \text{sgn}(v_i), \quad (2.8)$$

$$g(v_i) = \begin{cases} |1 + \frac{1}{v_i}|^{1/3} - |1 - \frac{1}{v_i}|^{1/3} & \text{if } v_i \neq 0, \\ 0 & \text{if } v_i = 0. \end{cases} \quad (2.9)$$

Let us note that the operator $\hat{\Theta}_i$ leaves invariant the Hilbert subspaces $\mathcal{H}_{\varepsilon_i}^{\pm}$ defined as the Cauchy completions with respect to the discrete inner product of the spaces

$$\text{Cyl}_{\varepsilon_i}^{\pm} = \text{span}\{|v_i\rangle; v_i \in \mathcal{L}_{\varepsilon_i}^{\pm}\}, \quad (2.10)$$

where $\mathcal{L}_{\varepsilon_i}^{\pm}$ are the semilattices of step two

$$\mathcal{L}_{\varepsilon_i}^{\pm} = \{\pm(\varepsilon_i + 2n), n = 0, 1, 2, \dots\}, \quad \varepsilon_i \in (0, 2]. \quad (2.11)$$

Therefore the constraint $\hat{C}_{\text{BI}}$ superselects the kinematical Hilbert space in different separable sectors. If we choose, for instance, a positive orientation for the triad in the three fiducial directions, we can restrict our study to the kinematical Hilbert space $\mathcal{H}_{\vec{\varepsilon}}^+ = \otimes_i \mathcal{H}_{\varepsilon_i}^+$, with $\vec{\varepsilon} = (\varepsilon_1, \varepsilon_2, \varepsilon_3)$.

C. Physical Hilbert space

In order to obtain the physical Hilbert space, it is enough to analyze the spectral properties of the operator $\hat{\Theta}_i$. It can be proven essentially self-adjoint with domain the dense set $\text{Cyl}_{\varepsilon_i}^+$. In consequence, $\hat{C}_{\text{BI}}$ is essentially self-adjoint in the invariant domain $\text{Cyl}_{\vec{\varepsilon}}^+ = \otimes_i \text{Cyl}_{\varepsilon_i}^+$. This property al-

allows us to apply the group averaging method [29,30] to determine the physical Hilbert space $\mathcal{H}_{\varepsilon}^{\text{Phys}}$.

In addition, the spectrum of $\hat{\Theta}_i$ is absolutely continuous, coincides with the real line and is nondegenerate. Furthermore, the coefficients $e_{\omega_i}^{\varepsilon_i}(2n + \varepsilon_i)$ ($n \in \mathbb{N}^+$) of its generalized eigenfunctions with eigenvalue ω_i turn out to be determined just by the initial data $e_{\omega_i}^{\varepsilon_i}(\varepsilon_i)$ [see Ref. [9] for the explicit expression -Eq. (45)-].

These eigenfunctions are formed by two components, one of them with support in the semilattice of step four

$${}^{(4)}\mathcal{L}_{\varepsilon_i}^+ = \{(\varepsilon_i + 4n), n = 0, 1, 2, \dots\}$$

and the other in the displaced semilattice

$${}^{(4)}\mathcal{L}_{\varepsilon_i+2}^+ = \{(\varepsilon_i + 2 + 4n), n = 0, 1, 2, \dots\}.$$

Both of these components are generalized eigenfunctions with eigenvalue ω_i^2 of the operator $\hat{\Theta}_i^2$, which is proportional to the gravitational part of the densitized constraint in the isotropic case. These components have a relative phase of $\pm \pi/2$ and, hence, $e_{\omega_i}^{\varepsilon_i}(v_i)$ oscillates rapidly when v_i varies in the semilattice $\mathcal{L}_{\varepsilon_i}^+$.

Applying the group averaging procedure, we obtain the following form for the wave function of the physical states

$$\Phi(\vec{v}) = \int_{\mathbb{R}^2} d\omega_2 d\omega_3 \tilde{\Phi}(\omega_2, \omega_3) e_{\omega_1(\omega_2, \omega_3)}^{\varepsilon_1}(v_1) e_{\omega_2}^{\varepsilon_2}(v_2) e_{\omega_3}^{\varepsilon_3}(v_3), \quad (2.12)$$

with

$$\omega_1(\omega_2, \omega_3) = -\frac{\omega_2 \omega_3}{\omega_2 + \omega_3}. \quad (2.13)$$

Here $\tilde{\Phi}(\omega_2, \omega_3)$ belongs to the physical Hilbert space, which turns out to be

$$\mathcal{H}_{\varepsilon}^{\text{Phys}} = L^2(\mathbb{R}^2, |\omega_2 + \omega_3| d\omega_2 d\omega_3). \quad (2.14)$$

In what follows, unless otherwise specified, ω_1 will be the function $\omega_1(\omega_2, \omega_3)$ given in Eq. (2.13).

III. WHEELER-DEWITT ANALOG

In this section we will study the quantization of the vacuum Bianchi I model in the WDW approach formulated in terms of the connection coefficients, which will be treated in a standard (nonpolymeric) way.

A. Kinematics and scalar constraint

Like in the loop quantization, we will work in the triad representation. As kinematical Hilbert space of the WDW quantization we take $\mathcal{H}_{\text{Kin}} = \otimes_i \mathcal{H}_{\text{Kin}}^i$ with $\mathcal{H}_{\text{Kin}}^i = L^2(\mathbb{R}, dv_i)$ [31]. The measure is the usual Lebesgue measure, and not the discrete one. In this representation the operator $\hat{p}_i$ acts by multiplication by the factor $p_i = 3^{1/3} \Delta \text{sgn}(v_i) |v_i|^{2/3}$, just as in the loop quantization. On the other hand, we promote the connection coefficients to

derivative operators,

$$\hat{c}^i = i 3^{1/6} 2 |v_i|^{1/6} \partial_{v_i} |v_i|^{1/6}, \quad (3.1)$$

to preserve the Dirac rule $[\hat{c}^i, \hat{p}_j] = i \hbar \{c^i, p_j\}$.

We denote by $\hat{\Theta}_i$ the counterpart of the classical quantity $c^i p_i$ in the WDW quantum theory [defined on the Schwartz space $\mathcal{S}(\mathbb{R})$]. We choose for $\hat{\Theta}_i$ the symmetric factor ordering which is analog to that used in the loop quantization, to simplify the comparison with it:

$$\hat{\Theta}_i = i \sqrt{3} \Delta \sqrt{|v_i|} [\text{sgn}(v_i) \partial_{v_i} + \partial_{v_i} \text{sgn}(v_i)] \sqrt{|v_i|}. \quad (3.2)$$

It is well-defined in the distributional sense and can be rewritten in the simpler form $\hat{\Theta}_i = i \sqrt{3} \Delta (1 + 2v_i \partial_{v_i})$, where we have disregarded the noncontributing term $|v_i| \delta(v_i)$. Then, the WDW quantum counterpart of the classical densitized Hamiltonian constraint can be constructed exclusively from the operator $\hat{\Theta}_i$ in the following manner

$$\hat{\mathcal{C}}_{\text{BI}} = -\frac{2}{\gamma^2} [\hat{\Theta}_1 \hat{\Theta}_2 + \hat{\Theta}_1 \hat{\Theta}_3 + \hat{\Theta}_2 \hat{\Theta}_3]. \quad (3.3)$$

The operator $\hat{\Theta}_i$ is essentially self-adjoint on $\mathcal{H}_{\text{Kin}}^i$. Furthermore, its restrictions to each of the subspaces $\mathcal{H}_{\text{Kin}}^{i,\pm} = L^2(\mathbb{R}^{\pm}, dv_i)$ are essentially self-adjoint as well. On each of these subspaces, the spectrum of $\hat{\Theta}_i$ is absolutely continuous, coincides with the real line and is nondegenerate, as happens to be the case with its analog $\hat{\Theta}_i$ in the loop quantization. Moreover, its generalized eigenfunctions, with generalized eigenvalue ω_i , have the form

$$\underline{e}_{\omega_i}(v_i) = \frac{1}{\sqrt{2\pi\alpha|v_i|}} \exp\left(-i\omega_i \frac{\ln|v_i|}{\alpha}\right), \quad (3.4)$$

where $\alpha = 2\sqrt{3}\Delta = 12\pi\gamma l_{\text{Pl}}^2$. They provide an orthonormal basis for $\mathcal{H}_{\text{Kin}}^{i,\pm}$. In analogy with the procedure followed in the loop quantization, we will restrict the study to $\mathcal{H}_{\text{Kin}}^+ = \otimes_i \mathcal{H}_{\text{Kin}}^{i,+}$.

B. Physical Hilbert space and observables

In order to obtain the physical Hilbert space, we apply the group averaging method like in the loop quantization. Obviously, the physical Hilbert space obtained is

$$\mathcal{H}^{\text{Phys}} = L^2(\mathbb{R}^2, |\omega_2 + \omega_3| d\omega_2 d\omega_3). \quad (3.5)$$

The wave function of the physical states has the following form:

$$\Phi(\vec{v}) = \int_{\mathbb{R}^2} d\omega_2 d\omega_3 \tilde{\Phi}(\omega_2, \omega_3) \underline{e}_{\omega_1}(v_1) \underline{e}_{\omega_2}(v_2) \underline{e}_{\omega_3}(v_3), \quad (3.6)$$

with $\tilde{\Phi}(\omega_2, \omega_3) \in \mathcal{H}^{\text{Phys}}$.

As in the LQC model [9], the operators $\hat{\Theta}_a$ (here $a = 2, 3$), which multiply the wave function by ω_a , together with $-i|\omega_2 + \omega_3|^{-1/2}\partial_{\omega_a}|\omega_2 + \omega_3|^{1/2}$, provide a complete set of observables, which are essentially self-adjoint operators on the domain $\mathcal{S}(\mathbb{R}^2) \subset \mathcal{H}^{\text{Phys}}$. Nonetheless, while the first pair are Dirac observables which correspond to classical constants of motion, the second one are not. As a consequence, this set turns out not to be adequate to introduce a nontrivial concept of evolution. In the next subsection, we will construct another pair of Dirac observables that will complete the set formed by $\hat{\Theta}_a$ ($a = 2, 3$), and in terms of which we will be able to develop an interpretation for the notion of evolution.

C. The evolution

In any gravitational system, as the one considered here, the Hamiltonian is constrained to vanish. Therefore, there is no well-defined notion of evolution in the model. Nonetheless, one can try to select, in the configuration space, a coordinate t (an internal time) and define a map between Hilbert spaces $\mathcal{H}_t$, where t takes values in a certain set $\mathcal{U}$ and $\mathcal{H}_t$ is the space of “initial data” given by the restriction of the wave function to the surface $t = \text{const}$. If there exists a unitary transformation $P_t: \mathcal{H}^{\text{Phys}} \rightarrow \mathcal{H}_t$, then each t -slice contains all the information needed to determine the physical state (i.e. the system is closed). Furthermore, if, in addition, the “identity” map between the spaces $\mathcal{H}_t$ (given by the trivial identification of data at different times) is also unitary, one can define a unitary evolution in $\mathcal{H}_t$. This is achieved by composing the inverse transformation P_t^{-1} , a transformation in the family P_t (for a different value of t), and the above identification of data.

In our case, since classically any of the three triad components is monotonous along all the dynamical trajectories, one can select one of the v_i 's as an internal time. Taking into account that in the description of the physical states (3.6) we have already eliminated ω_1 in terms of ω_2 and ω_3 , it is then most natural to choose $t := v_1$.

We can easily introduce the initial data spaces labeled by $v_1 = \text{const}$ (which we will also call “slice” spaces) via the transformation

$$\begin{aligned}\Phi_{v_1}(v_2, v_3) &= \int_{\mathbb{R}^2} d\omega_2 d\omega_3 \tilde{\Phi}_{v_1}(\omega_2, \omega_3) \underline{e}_{\omega_2}(v_2) \underline{e}_{\omega_3}(v_3), \\ \tilde{\Phi}_{v_1}(\omega_2, \omega_3) &:= P_{v_1} \tilde{\Phi}(\omega_2, \omega_3) := \tilde{\Phi}(\omega_2, \omega_3) \underline{e}_{\omega_1}(v_1),\end{aligned}\quad (3.7)$$

with $\tilde{\Phi}_{v_1}(\omega_2, \omega_3)$ belonging to

$$\begin{aligned}\mathcal{H}_{v_1} &= L^2(\mathbb{R}^2, |\omega_2 + \omega_3| \underline{e}_{\omega_1}(v_1)^{-2} d\omega_2 d\omega_3) \\ &= L^2(\mathbb{R}^2, 2\pi\alpha v_1 |\omega_2 + \omega_3| d\omega_2 d\omega_3).\end{aligned}\quad (3.8)$$

Since $\underline{e}_{\omega_1}(v_1)$, given in Eq. (3.4), never vanishes, all the slice spaces $\mathcal{H}_{v_1}$ are unitarily related to $\mathcal{H}^{\text{Phys}}$.

Introducing an additional rescaling one can define the alternate transformation

$$\begin{aligned}\Phi_{v_1}(v_2, v_3) &= \int_{\mathbb{R}^2} \frac{d\omega_2 d\omega_3}{\sqrt{2\pi\alpha v_1}} \tilde{\Phi}'_{v_1}(\omega_2, \omega_3) \underline{e}_{\omega_2}(v_2) \underline{e}_{\omega_3}(v_3), \\ \tilde{\Phi}'_{v_1}(\omega_2, \omega_3) &:= P'_{v_1} \tilde{\Phi}(\omega_2, \omega_3) \\ &:= \tilde{\Phi}(\omega_2, \omega_3) \sqrt{2\pi\alpha v_1} \underline{e}_{\omega_1}(v_1) \in \mathcal{H}'_{v_1},\end{aligned}\quad (3.9)$$

where

$$P'_{v_1}: \mathcal{H}^{\text{Phys}} \rightarrow \mathcal{H}'_{v_1} \quad (3.10a)$$

$$\mathcal{H}'_{v_1} = L^2(\mathbb{R}^2, |\omega_2 + \omega_3| d\omega_2 d\omega_3). \quad (3.10b)$$

Since P'_{v_1} is unitary and the spaces $\mathcal{H}'_{v_1}$ coincide (so that the corresponding map identifying states at different values of v_1 is unitary as well), it is clear that P'_{v_1} leads to a unitary evolution for the system.

A more elaborated manner of providing a concept of evolution is by introducing a family of *partial observables* [32,33], which are to be related via unitary transformations. A natural construction of partial observables from the kinematical ones is available if there exists an internal time which provides a unitary map between initial data spaces. On the formal level, one can do this through the group averaging procedure. Alternatively, if there exists a decomposition $\mathcal{H}_{\text{Kin}} = \mathcal{H}^t \otimes \mathcal{H}'$ (where $\mathcal{H}^t$ is some Hilbert space of functions depending on t only) [34] and there is an operator $\hat{O}': \mathcal{H}' \rightarrow \mathcal{H}'$, one can build $\hat{O}_t$ (which measures the corresponding quantity “at a given time t ”) as an operator whose action is defined through the following sequence of operations:

- (i) Take an initial data slice $\psi_t \in \mathcal{H}_t$ corresponding to the value t of an emergent time. In many cases the spaces $\mathcal{H}_t$ differ from $\mathcal{H}'$. Therefore one has to define a transformation $\mathcal{H}_t \rightarrow \mathcal{H}'$ [35].
- (ii) Then act with the “kinematical” observable $\hat{O}'$ corresponding to the measured quantity, and
- (iii) use the relation between physical and slice Hilbert spaces to find the element of $\mathcal{H}^{\text{Phys}}$ corresponding to the result of (ii).

In the model under study, the above method can be applied, for example, to the kinematical observable $\ln(\hat{v}_a)$ (where $a = 2, 3$), which acts on elements of $\mathcal{H}_{\text{Kin}}^{a,+}$ as a multiplication operator. As the internal time coordinate we still choose v_1 , so that $\mathcal{H}_t := \mathcal{H}_{v_1}$, given by Eq. (3.8). The space $\mathcal{H}'$ is the product

$$\mathcal{H}' := \mathcal{H}_{\text{Kin}}^{2,+} \otimes \mathcal{H}_{\text{Kin}}^{3,+} = L^2((\mathbb{R}^+)^2, dv_2 dv_3). \quad (3.11)$$

Since $\mathcal{H}_{v_1}$ and $\mathcal{H}'$ are different, we introduce a unitary transformation $\mathcal{H}_{v_1} \rightarrow \mathcal{H}'$. In the corresponding ω_a -representations, it is given by the map

$$\begin{aligned}\tilde{\Phi}_{v_1}(\omega_2, \omega_3) &\mapsto \tilde{\chi}_{v_1}(\omega_2, \omega_3) \\ &:= \sqrt{2\pi\alpha v_1} |\omega_2 + \omega_3|^{1/2} \tilde{\Phi}_{v_1}(\omega_2, \omega_3).\end{aligned}\quad (3.12)$$

In the v_a -representation, this transformation is simply the map $\Phi_{v_1}(v_2, v_3) \rightarrow \chi_{v_1}(v_2, v_3)$, with $\Phi_{v_1}(v_2, v_3)$ given in the first line of Eq. (3.7) and

$$\chi_{v_1}(v_2, v_3) = \int_{\mathbb{R}^2} d\omega_2 d\omega_3 \tilde{\chi}_{v_1}(\omega_2, \omega_3) \underline{e}_{\omega_2}(v_2) \underline{e}_{\omega_3}(v_3). \quad (3.13)$$

Employing the transformations between the introduced Hilbert spaces, we finally obtain a family of observables $\ln(\hat{v}_a)_{v_1}$ acting on the physical Hilbert space, interpretable as “the value of $\ln(v_a)$ at the fixed time v_1 ”. The operators are well-defined on the Schwartz space $\mathcal{S}(\mathbb{R}^2)$. Their action in this domain, which can be deduced taking into account that they act by multiplication on the corresponding kinematical states $\chi_{v_1}(v_2, v_3)$, turns out to be

$$\begin{aligned}[\ln(\hat{v}_a)_{v_1} \tilde{\Phi}](\omega_2, \omega_3) &= \frac{-i\alpha}{\underline{e}_{\omega_1}(v_1)} |\omega_2 + \omega_3|^{-1/2} (\partial_{\omega_a}) \\ &\times [|\omega_2 + \omega_3|^{1/2} \tilde{\Phi}(\omega_2, \omega_3) \underline{e}_{\omega_1}(v_1)].\end{aligned}\quad (3.14)$$

The observables $\ln(\hat{v}_a)_{v_1}$, together with the constants of motion $\hat{\underline{Q}}_a|_{v_1} := \hat{\underline{Q}}_a$, form a complete set of Dirac observables. Whereas within each family (corresponding to $a = 2, 3$, respectively) the observables $\hat{\underline{Q}}_a|_{v_1}$ do not change with v_1 , the observables $\ln(\hat{v}_a)_{v_1}$ do not coincide, and are related at different times v_1 and v_1^* via an operator $\hat{\underline{Q}}_{v_1, v_1^*}: \mathcal{H}^{\text{Phys}} \rightarrow \mathcal{H}^{\text{Phys}}$ such that

$$[\hat{\underline{Q}}_{v_1, v_1^*} \tilde{\Phi}](\omega_2, \omega_3) = \sqrt{\frac{v_1 \underline{e}_{\omega_1}(v_1)}{v_1^* \underline{e}_{\omega_1}(v_1^*)}} \tilde{\Phi}(\omega_2, \omega_3). \quad (3.15)$$

The form of the eigenfunction (3.4) implies immediately, that these operators are both invertible ($\hat{\underline{Q}}_{v_1, v_1^*}^{-1} = \hat{\underline{Q}}_{v_1^*, v_1}$) and unitary on $\mathcal{H}^{\text{Phys}}$. Therefore, the relation between observables at different times,

$$\ln(\hat{v}_a)_{v_1^*} = \hat{\underline{Q}}_{v_1, v_1^*} \ln(\hat{v}_a)_{v_1} \hat{\underline{Q}}_{v_1^*, v_1}, \quad (3.16)$$

is unitary.

As a consequence, the families of observables $\ln(\hat{v}_a)_{v_1}$ define on the physical Hilbert space $\mathcal{H}^{\text{Phys}}$ a unitary evolution that is local in the emergent time v_1 . In contrast, as we will see in Sec. VB, the direct application of the above construction in the loop quantization does not lead to a unitary evolution since, in that case, the analogs of $\hat{\underline{Q}}_{v_1, v_1^*}$ fail to be unitary operators. Nonetheless (as we will see in Sec. VIB) families of unitarily related observables can be defined once we use, instead of v_1 , its conjugate momen-

tum, denoted by b_1 , which provides a suitable emergent time in the loop quantization.

To compare the dynamics predicted by the constructed families of observables with the classical dynamics, let us calculate the expectation values on some class of states which are semiclassical at late times, namely, Gaussian states peaked around large values of ω_2^* and ω_3^* :

$$\tilde{\Phi}(\omega_2, \omega_3) = \frac{K}{\sqrt{|\omega_2 + \omega_3|}} \prod_{a=2}^3 e^{-(\omega_a - \omega_a^*)^2 / (2\sigma_a^2)} e^{i\beta^a \omega_a}, \quad (3.17)$$

where K is a normalization factor such that $\|\tilde{\Phi}\| = 1$, and the factor $|\omega_2 + \omega_3|^{-1/2}$ compensates the nontrivial factor in the measure of the physical Hilbert space (3.5).

For a general state $\tilde{\Phi}$, using directly the explicit form of the observables (3.14) and integrating the inner product, we find that

$$\langle \tilde{\Phi} | \ln(\hat{v}_a)_{v_1} \tilde{\Phi} \rangle = A_a \ln v_1 + B_a, \quad (3.18)$$

where the constant coefficients A_a and B_a are

$$A_a = \|\omega_1(\omega_2, \omega_3) \omega_a^{-1} \tilde{\Phi}\|^2, \quad (3.19a)$$

$$B_a = \alpha \langle \tilde{\Phi} | |\omega_2 + \omega_3|^{-1/2} (-i\partial_{\omega_a}) |\omega_2 + \omega_3|^{1/2} \tilde{\Phi} \rangle. \quad (3.19b)$$

Evaluating them for the Gaussian form (3.17) of $\tilde{\Phi}$ and taking the limit $\sigma_a \rightarrow 0$ (for both $a = 2, 3$), we obtain the following trajectory

$$\langle \tilde{\Phi} | \ln(\hat{v}_a)_{v_1} \tilde{\Phi} \rangle = \left[\frac{\omega_1(\omega_2^*, \omega_3^*)}{\omega_a^*} \right]^2 \ln v_1 + \alpha \beta^a \quad (3.20)$$

which agrees with the classical one. This result implies that in the WDW theory the singularities of the vacuum Bianchi I universe are not resolved dynamically (in the sense of the trajectories defined by the expectation values on semiclassical states). Actually, the lack of singularity resolution is a general property of all the states for which the coefficients A_a and B_a defined in Eq. (3.19) are finite.

To analyze the behavior of the dispersions $\langle \Delta \ln(\hat{v}_a)_{v_1} \rangle$, we first find the expectation values of $\ln^2(\hat{v}_a)_{v_1}$ in a way similar to the derivation of Eq. (3.18). They read

$$\langle \tilde{\Phi} | \ln^2(\hat{v}_a)_{v_1} \tilde{\Phi} \rangle = W_a \ln^2 v_1 + Y_a \ln v_1 + X_a, \quad (3.21)$$

where

$$W_a = \|\omega_1^2(\omega_2, \omega_3) \omega_a^{-2} \tilde{\Phi}\|^2, \quad (3.22a)$$

$$\begin{aligned}Y_a &= -2i\alpha \langle \tilde{\Phi} | |\omega_2 + \omega_3|^{-1/2} \omega_1(\omega_2, \omega_3) \omega_a^{-1} (\partial_{\omega_a}) \\ &\times |\omega_2 + \omega_3|^{1/2} \omega_1(\omega_2, \omega_3) \omega_a^{-1} \tilde{\Phi} \rangle,\end{aligned}\quad (3.22b)$$

$$X_a = -\alpha^2 \langle \tilde{\Phi} | |\omega_2 + \omega_3|^{-1/2} \partial_{\omega_a}^2 |\omega_2 + \omega_3|^{1/2} \tilde{\Phi} \rangle. \quad (3.22c)$$

In Eq. (3.22b), there is no summation over the indices a . Using the standard relation $\langle \Delta \ln(\hat{v}_a)_{v_1} \rangle^2 = \langle \ln(\hat{v}_a)_{v_1}^2 \rangle - \langle \ln(\hat{v}_a)_{v_1} \rangle^2$ we can easily find the dispersions. In particular,

we see immediately that once these dispersions are finite in some epoch, they remain so throughout all the evolution. Furthermore, for states for which the expectation values B_a and X_a [defined in Eqs. (3.19) and (3.22)] are finite, the relative dispersions approach constant values in the large v_1 limit, values which are determined by the relative dispersions of $\omega_1^2(\omega_2, \omega_3)\omega_a^{-2}$:

$$\lim_{v_1 \rightarrow \infty} \frac{\langle \Delta \ln(\hat{v}_a)_{v_1} \rangle}{\langle \ln(\hat{v}_a)_{v_1} \rangle} = \frac{\langle \Delta[\omega_1^2(\omega_2, \omega_3)\omega_a^{-2}] \rangle}{\langle \omega_1^2(\omega_2, \omega_3)\omega_a^{-2} \rangle}. \quad (3.23)$$

Here we have used the shorthand $\langle \hat{O} \rangle := \langle \hat{\Phi} | \hat{O} | \hat{\Phi} \rangle$ for any operator $\hat{O}$.

D. b -representation

In the loop quantization, the evolution with respect to the internal time v_1 , analog to the one constructed above for the WDW theory, fails to be unitary. Nevertheless, the use of the momentum conjugate to v_1 as internal time provides a good notion of unitary evolution. Let us study this choice of time in the WDW quantization as well, both for completeness and in order to introduce the procedure in a simple setting, where the difficulties inherent to the more complicated nature of the LQC model are absent.

Given the classical variable v_i introduced in Eq. (2.3), one can define the conjugate momentum

$$b_i := \sqrt{\Delta} c^i |p_i|^{-1/2}, \quad (3.24)$$

such that

$$\{b_i, v_j\} = 2\delta_{ij}. \quad (3.25)$$

In the WDW quantum theory, the unitary transformation between the “position” and “momentum” representations is given by the Fourier transform:

$$[\mathcal{F}\psi](b_i) = \frac{1}{2\sqrt{\pi}} \int_{\mathbb{R}} dv_i \psi(v_i) e^{-(i/2)v_i b_i}. \quad (3.26)$$

It is worth emphasizing that this is a unitary transformation from the Hilbert space of square integrable functions in the v_i -representation to the *same Hilbert space* in the b_i -representation:

$$\mathcal{F}: \mathcal{H}_{\text{Kin}}^i = L^2(\mathbb{R}, dv_i) \rightarrow \tilde{\mathcal{H}}_{\text{Kin}}^i = L^2(\mathbb{R}, db_i). \quad (3.27)$$

Under this transformation the elementary kinematical operators transform as

$$\hat{v}_i \rightarrow 2i\partial_{b_i}, \quad \partial_{v_i} \rightarrow i\hat{b}_i/2, \quad (3.28)$$

where $\hat{b}_i$ acts in the new representation as a multiplication operator. Hence, the transformed of $\hat{\Theta}_i$ is

$$\mathcal{F}(\hat{\Theta}_i) = -i\sqrt{3}\Delta(1 + 2b_i\partial_{b_i}), \quad (3.29)$$

which coincides with the original operator $\hat{\Theta}_i$ (up to a sign), both being defined in identical Hilbert spaces. Therefore, in the WDW quantum theory, working in the

b_i -representation is completely equivalent to working in the v_i -representation. In particular, we can regard b_1 as the internal time, change the representation only in the direction 1, and define the Hamiltonian constraint in the kinematical Hilbert space $\tilde{\mathcal{H}}_{\text{Kin}}^{1,+} \otimes_a \mathcal{H}_{\text{Kin}}^{a,+}$ ($a = 2, 3$), where $\tilde{\mathcal{H}}_{\text{Kin}}^{1,+} = L^2(\mathbb{R}^+, db_1)$ [36], by replacing the operator $\hat{\Theta}_1$ with the operator $\mathcal{F}(\hat{\Theta}_1)$ in Eq. (3.3). Hence, we can repeat exactly the construction introduced in Sec. III C substituting v_1 by b_1 and $\underline{e}_{\omega_1}(v_1)$ by $\underline{e}_{-\omega_1}(b_1)$.

Whereas the b_i -representation does not introduce any novelty or advantage in the WDW quantization in comparison with the v_i -representation, we will see in Sec. VI that there is a big difference between both approaches in the LQC quantization.

IV. WHEELER-DEWITT LIMIT OF THE LOOP STATES

The comparison of Eqs. (3.5) and (3.6) with Eqs. (2.12), (2.13), and (2.14) shows that the physical Hilbert spaces of the LQC and WDW quantizations, as well as the structure of the corresponding wave functions, are identical. The difference between both quantizations is captured in the different form that the eigenfunctions of the operators $\hat{\Theta}_i$ and $\hat{\Theta}_i$ possess. On the other hand (as it will be shown in Sec. IVA), the LQC eigenfunctions converge for large v_i to some combinations of their WDW analogs. This feature allows one to regard the dynamics of the LQC universe as certain form of “scattering” of WDW states, incoming from a distant past and outgoing to a distant future [37]. Mathematically, this behavior is described by the analog of a scattering matrix $\hat{\rho}_s$ acting on the incoming WDW state:

$$|\Phi\rangle_{\text{out}} = \hat{\rho}_s |\Phi\rangle_{\text{in}}, \quad (4.1a)$$

$$(\underline{e}_{\omega_2}, \underline{e}_{\omega_3} | \hat{\rho}_s | \underline{e}_{\omega'_2}, \underline{e}_{\omega'_3}) = \hat{\rho}_1(\omega_1(\omega_2, \omega_3), \omega_1(\omega'_2, \omega'_3)) \times \hat{\rho}_2(\omega_2, \omega'_2) \hat{\rho}_3(\omega_3, \omega'_3), \quad (4.1b)$$

$$\hat{\rho}_i(\omega_i, \omega'_i) := (\underline{e}_{\omega_i} | \hat{\rho}_i | \underline{e}_{\omega'_i}). \quad (4.1c)$$

In turn, the matrices $\hat{\rho}_i$ are determined by the WDW limit of the eigenfunctions of $\hat{\Theta}_i$. The exact form of this limit will be investigated in Sec. IVA. The result will be applied in Sec. IV B to describe the limit of physical states. Finally, Sec. IV C deals with the effect of the commented scattering on the dispersion of observables.

A. Limit of the eigenfunctions

Let us restrict ourselves to one superselection sector (defined in Sec. II C), e.g. that corresponding to functions supported on the lattice $\mathcal{L}_{\varepsilon_i}^+$. The eigenfunctions $e_{\omega_i}^{\varepsilon_i}$ of $\hat{\Theta}_i$ with eigenvalue ω_i were provided already in Ref. [9] [see Eq. (45)], although in the form presented there one cannot easily determine their large v_i behavior. In order to find it, we have to analyze the operator $\hat{\Theta}_i$ itself. Its properties were discussed in detail in Ref. [9] as part of the proof of its

self-adjointness. First, all of its eigenspaces are one-dimensional, and the complete solution is determined by an initial value $e_{\omega_i}^{\varepsilon_i}(\varepsilon_i)$. In particular, the freedom in the choice of a global phase for the eigenfunctions is removed by demanding the positivity of this initial value $e_{\omega_i}^{\varepsilon_i}(\varepsilon_i)$. Second, as discussed in Sec. II C, one can split the support into two subsemilattices $^{(4)}\mathcal{L}_{\tilde{\varepsilon}_i}^+$, with $\tilde{\varepsilon}_i \in \{\varepsilon_i, \varepsilon_i + 2\}$. The restriction of $e_{\omega_i}^{\varepsilon_i}$ to each subsemilattice is an eigenfunction of the operator $\hat{\Theta}_i^2$ with eigenvalue ω_i^2 :

$$\hat{\Theta}_i^2 e_{\omega_i}^{\tilde{\varepsilon}_i} = \omega_i^2 e_{\omega_i}^{\tilde{\varepsilon}_i}, \quad e_{\omega_i}^{\tilde{\varepsilon}_i} := e_{\omega_i}^{\varepsilon_i}|_{^{(4)}\mathcal{L}_{\tilde{\varepsilon}_i}^+}. \quad (4.2)$$

The operator $\hat{\Theta}_i^2$, in turn, is a second order difference operator with real coefficients (similar in structure to the evolution operator defined in Ref. [5]). It also has the property that all its eigenspaces are one-dimensional and the eigenfunctions are determined just by their initial value (at $v_i = \tilde{\varepsilon}_i$).

To check the existence of the WDW limit of the eigenfunctions, we implement the method used in Ref. [38]:

- (i) First, we represent the values of the eigenfunction at two consecutive points of $^{(4)}\mathcal{L}_{\tilde{\varepsilon}_i}^+$ by vectors $\vec{\psi}(v)$ of coefficients of its decomposition in terms of the WDW eigenfunctions $\underline{e}_{\pm|\omega_i|}$ evaluated at this pair of points.
- (ii) Next, we rewrite the eigenfunction equation as the first order one acting on the vectors $\vec{\psi}(v)$. It has a form of a 2×2 matrix [denoted from now on as $\mathbf{B}(v)$].
- (iii) Finally, we calculate the asymptotic expansion of the matrix $\mathbf{B}$ in the large v limit.

An explicit calculation shows that the considered matrix is of the form $\mathbf{B}(v) = \mathbb{I} + \mathcal{O}(v^{-2})$. Thus, there exists a well-defined limit

$$\vec{\psi} := \lim_{v \rightarrow \infty} \vec{\psi}(v). \quad (4.3)$$

This immediately implies the convergence to a combination of functions in the WDW basis, represented by the coefficient vector $\vec{\psi}$. The form of $\mathbf{B}$ implies also that the rate of convergence of $\vec{\psi}(v)$ is at least of order $1/v$.

Actually, the fact that the operator $\hat{\Theta}_i^2$, after a suitable change of representation, differs from the isotropic evolution operator of Ref. [5] just by a compact term (see Ref. [9]) allows us to apply here the numerical results of that reference. They show that the convergence is even faster, namely

$$\vec{\psi}(v) = \vec{\psi} + \mathcal{O}(v^{-5/2}). \quad (4.4)$$

Furthermore, from the reality of $\hat{\Theta}_i^2$, it follows that the incoming and outgoing WDW plane waves contribute equally to the limit, that is

$$\vec{\psi} = r \begin{bmatrix} e^{i\phi(\omega_i)} \\ e^{-i\phi(\omega_i)} \end{bmatrix}. \quad (4.5)$$

To determine the normalization factor r we note that $\lim_{v \rightarrow \infty} (\partial_v \underline{e}_{\omega_i}(v)) / \underline{e}_{\omega_i}(v) = 0$. This fact, together with the sufficiently fast rate of convergence (4.4), imply that the (kinematical) norms of both $e_{\omega_i}^{\tilde{\varepsilon}_i}$ and its WDW limit (denoted here as $\underline{e}_{\omega_i}^{\tilde{\varepsilon}_i}$) satisfy the relation $8\|e_{\omega_i}^{\tilde{\varepsilon}_i}\|^2 = \|\underline{e}_{\omega_i}^{\tilde{\varepsilon}_i}\|^2$. As a consequence

$$r(\omega_i) = \sqrt{2}z_i, \quad (4.6)$$

where z_i is a global phase which equals 1 for $\tilde{\varepsilon}_i \leq 2$ and $-i \operatorname{sgn}(\omega_i)$ otherwise.

The phase shift $\phi(\omega_i)$ has a nontrivial dependence on ω_i and needs to be found numerically. Luckily, the similarity of the operator $\hat{\Theta}_i^2$ with the evolution operator of an isotropic universe allows us again to apply directly the methods of Ref. [37]. The result is the following:

$$\phi(\omega_i) = (\ln|\omega_i| + a)(|\omega_i| + b) + c_{\tilde{\varepsilon}_i} + R_{\tilde{\varepsilon}_i}(|\omega_i|), \quad (4.7)$$

where a , b and $c_{\tilde{\varepsilon}_i}$ are constants, $\lim_{\omega_i \rightarrow \infty} R_{\tilde{\varepsilon}_i}(|\omega_i|) = 0$, and the dependence on $\tilde{\varepsilon}_i$ enters only in the constant term and in the remnant part. Hence, for large $|\omega_i|$ the terms that affect the position and dispersion of the wave packet do not depend on the value of $\tilde{\varepsilon}_i$.

At this point, we can already write the exact form of the scattering matrix $\hat{\rho}_i$ defined for just one subsemilattice. It reads:

$$\hat{\rho}_i(\omega_i, \omega'_i) = e^{-2i\phi(\omega_i)} \delta(\omega_i + \omega'_i). \quad (4.8)$$

Let us remember that the parts supported on different subsemilattices (individually of constant phase) are shifted in phase by $\pi/2$. As a consequence, the common WDW limit for both of them does not exist (see Fig. 1). Therefore, one cannot write an explicit form for the scattering matrix $\hat{\rho}_i$ on the entire lattice $\mathcal{L}_{\tilde{\varepsilon}_i}^+$. Nonetheless, the differences between subsemilattices manifest themselves only through the constant phase shift and the remnant decaying for large ω_i . As a consequence, when we consider the properties of asymptotic wave packets, peaked around large ω_a , we can safely restrict the studies just to one subsemilattice.

B. Physical states

The WDW limit of the eigenfunctions found in the previous subsection can be now applied in the analysis of the physical states. We start with a general state $\tilde{\Phi}$, again restricting the study just to particular subsemilattices $^{(4)}\mathcal{L}_{\tilde{\varepsilon}_i}^+$. In order to find the limit of the corresponding wave function, we simply replace the basis functions $e_{\omega_i}^{\tilde{\varepsilon}_i}$ in Eq. (2.12) with their large v_i limits

$$e_{\omega_i}^{\tilde{\varepsilon}_i} \rightarrow r[e^{i\phi(\omega_i)} \underline{e}_{\omega_i} + e^{-i\phi(\omega_i)} \underline{e}_{-\omega_i}]. \quad (4.9)$$

Upon this replacement, the wave function $\Phi(\vec{v})$ is trans-

FIG. 1 (color online). An example of eigenfunction of the operator $\hat{\Theta}_i$, corresponding to the eigenvalue $\omega_i = 100$ and the superselection sector $\varepsilon_i = 2$. The blue line (located on the imaginary plane) shows the part supported on the subsemilattice $^{(4)}\mathcal{L}_{\tilde{\varepsilon}_i=4}^+$, whereas the red line (real plane) is the part supported on $^{(4)}\mathcal{L}_{\tilde{\varepsilon}_i=2}^+$.

formed into the function

$$\begin{aligned} \underline{\Phi}(\vec{v}) = & \sum_{s_2, s_3 = \pm 1} \int_{\mathbb{R}^2} d\omega_2 d\omega_3 \tilde{\Phi}_{\vec{s}}(\omega_2, \omega_3) \underline{e}_{\omega_{\vec{s}}(\omega_2, \omega_3)}(v_1) \\ & \times \underline{e}_{\omega_2}(v_2) \underline{e}_{\omega_3}(v_3), \end{aligned} \quad (4.10)$$

where $\vec{s} := (s_2, s_3)$, $\omega_{\vec{s}}(\omega_2, \omega_3) := \omega_1(s_2\omega_2, s_3\omega_3)$, and

$$\begin{aligned} \tilde{\Phi}_{\vec{s}}(\omega_2, \omega_3) = & 2\sqrt{2} \sum_{s_1 = \pm 1} \tilde{\Phi}(s_1 s_2 \omega_2, s_1 s_3 \omega_3) e^{is_1 \phi(\omega_{s_1 \vec{s}})} \\ & \times s_1^{(3-z_1^2-z_2^2-z_3^2)/2} \prod_{a=2}^3 s_a^{(1-z_a^2)/2} \\ & \times z_a e^{is_1 s_a \phi(s_1 s_a \omega_a)}, \end{aligned} \quad (4.11)$$

where z_i^2 equals 1 for $\tilde{\varepsilon}_i \leq 2$ and -1 otherwise. Note that, in order to obtain the above expression, we have taken into account that $\omega_1(-\omega_2, -\omega_3) = -\omega_1(\omega_2, \omega_3)$ and $r(s_j \omega_i) = s_j^{(1-z_i^2)/2} \sqrt{2} z_i$ (with $\omega_1 = \omega_{\vec{s}}$).

If we compare Eq. (4.10) with Eq. (3.6) we see that each term, corresponding to a particular set of values of s_a , has a form very similar to that of a WDW state with spectral profile $\underline{\Phi} = \tilde{\Phi}_{\vec{s}}$, the only difference being the replacement of the function ω_1 with $\omega_{\vec{s}}$ in the index of the basis functions. As a consequence, each of those terms can be (independently) considered as a state defined within a certain analog of the WDW quantum theory described in Sec. III. Such an analog inherits all the properties and structure of the original theory, except for the transformation of $\omega_1 \rightarrow \omega_{\vec{s}}$ pointed out above. In particular, the inner product and the definitions of all the observables remain unmodified.

This correspondence allows us to apply directly the definitions (3.14) of the observables $\ln(\hat{v}_a)_{v_1}$ to the terms $\tilde{\Phi}_{\vec{s}}$. Their expectation values (calculated on each term independently) satisfy an analog of the Eq. (3.18) with the direction coefficient A_a replaced with

$$A_{a,\vec{s}} := s_a \|\omega_{\vec{s}}(\omega_2, \omega_3) \omega_a^{-1} \tilde{\Phi}_{\vec{s}}\|^2. \quad (4.12)$$

To select the terms $\tilde{\Phi}_{\vec{s}}$ which actually contribute to the investigated limit we note that, if the state is localized (in the sense that it remains peaked around the trajectories defined by the expectation values of the considered observables), only those terms corresponding to an $\vec{s}$ for which $A_{a,\vec{s}}$ is strictly positive will have a significant contribution in the regime when the three v_i 's are all large. This requirement is satisfied only by the term with $s_2 = s_3 = 1$.

The surviving term encodes the state of the genuine (untransformed) WDW theory. Therefore, the large v_i limit of a localized state $\tilde{\Phi}$ is simply given by a WDW state of spectral profile

$$\begin{aligned} \underline{\tilde{\Phi}}(\omega_2, \omega_3) = & 2\sqrt{2} \sum_{s = \pm 1} s^{(3-z_1^2-z_2^2-z_3^2)/2} \tilde{\Phi}(s\omega_2, s\omega_3) \\ & \times \prod_{i=1}^3 z_i e^{is\phi(s\omega_i)}, \end{aligned} \quad (4.13)$$

where ω_1 is again related to ω_2 and ω_3 via Eq. (2.13).

Let us recall at this stage that the variable v_1 plays the role of time; therefore it is proper to introduce a decomposition of the state into positive and negative frequency parts, corresponding to $\omega_1 > 0$ and $\omega_1 < 0$ respectively. Physically, these components can be interpreted as moving forward and backward in time. An analog correspondence can be applied to other directions, defining the splitting into expanding and contracting components. Then, the change of sign in ω_a corresponds to a parity reflection in $x_a = \ln(v_a)$. As a consequence, the transformation $\{\omega_i\} \rightarrow \{-\omega_i\}$, which we have recognized as a symmetry of Eq. (2.13) in our previous discussion, is the analog of the full PT (parity/time inversion) transformation.

Let us now consider a LQC state with profile $\tilde{\Phi}(\omega_2, \omega_3)$ which is localized in the sense explained above, and restrict our considerations to the corresponding WDW state with profile $\underline{\tilde{\Phi}}(\omega_2, \omega_3)$. For convenience, in the following we will call $2\sqrt{2}\tilde{\Phi}(\omega_2, \omega_3)$ the *reference state*. The expectation values of $\ln(\hat{v}_a)_{v_1}$ follow then the trajectory (3.18) for some constants A_a and B_a . Furthermore, from Eq. (4.13), one can immediately see that the WDW state consists of two parts: one with the same parity/time orientation as the reference state ($s = 1$) and another which is PT reflected ($s = -1$). We denote them, respectively, by $\underline{\tilde{\Phi}}_+$ and $\underline{\tilde{\Phi}}_-$. If the reference state has a definite time orientation (only one sign of ω_1 contributes) then the distinguished components are, respectively, the part comoving in time with the reference state and the time-reflected part. Since the norms of

both of these components are equal, any wave packet moving backward in time is fully reflected into a packet moving forward. This shows the presence of a bounce also in the internal time direction.

In order to compare the trajectories of the expectation values of $\ln(\hat{v}_a)$ in the considered components with those of the reference state, we note that, since their spectral profiles are related just by a rotation, and by the reflection in ω_a together with a possible change of sign in the case of $\tilde{\Phi}_-$, the directional coefficients A_a are the same for these component states and the reference state. The only change is in the parameter B_a . As a consequence, the trajectories are just shifted with respect to the trajectory of the reference state.

In the particular case of Gaussian reference states which are sharply peaked around large ω_a^* ,

$$\tilde{\Phi}(\omega_2, \omega_3) = \frac{K}{\sqrt{|\omega_2 + \omega_3|}} \prod_{a=2}^3 e^{-(\omega_a - \omega_a^*)^2 / (2\sigma_a^2)} e^{i\beta^a \omega_a} \quad (4.14)$$

(where K is chosen so that $\tilde{\Phi}$ has unit norm), we can provide a quantitative estimation of the trajectory shift. Namely, for such states the phase rotation $\phi(\omega_i)$ is well approximated by its first order expansion (with coefficients D and E which depend on ω_i^*)

$$\begin{aligned} \phi(\omega_i) &\approx D(\omega_i^*)(\omega_i - \omega_i^*) + E(\omega_i^*), \\ D(\omega_i^*) &= \text{sgn}(\omega_i^*)(1 + a + \ln|\omega_i^*|), \end{aligned} \quad (4.15)$$

where a is the constant given in Eq. (4.7). In view of this approximation, one can almost directly repeat the calculations of Sec. III C to find the formula equivalent to Eq. (3.18). The resulting trajectories are

$$\begin{aligned} [\ln v_a](v_1) &= \left[\frac{\omega_1(\omega_2^*, \omega_3^*)}{\omega_a^*} \right]^2 [\ln v_1 - \alpha D(\omega_1^*)] \\ &+ \alpha [D(\omega_a^*) \pm \beta^a]. \end{aligned} \quad (4.16)$$

Generically, these trajectories are disjoint, both between them and with respect to the trajectory of the reference state. Nonetheless, note that the two considered trajectories coincide in the case $\beta^a = 0$.

C. The dispersions

In the discussion above, we have taken the limit $\sigma_a \rightarrow 0$ ($a = 2, 3$) and considered the linear approximation to the variation of the rotation phase $\phi(\omega_i)$. This essentially removes all the information about the behavior of the dispersions. However, in the scenario described in the previous subsection, where the LQC dynamics can be (in an asymptotic sense) viewed as the reflection of the WDW wave packet $\tilde{\Phi}_-$, which moves backward in time and is contracting, into the moving forward and expanding wave packet $\tilde{\Phi}_+$, it is important to ask how much the dispersion

of $\tilde{\Phi}_+$ grows in comparison to the one of $\tilde{\Phi}_-$ (or vice versa). For the isotropic model with massless scalar field, restrictive bounds on possible dispersion-growth have been found. This result can be extended by employing the exact triangle inequalities [37] which involve the dispersion in $\ln|\omega_a|$ and $\ln(\hat{v}_a)$ (for brevity, we suppress the subindex v_1 in the latter of these operators).

In the model considered here, given that the analysis of the WDW analog shows that the *relative* dispersions in $\ln(\hat{v}_a)$ are the ones which approach constant (nonzero) values for large v_1 [see Eq. (3.23)], we are interested in finding a weaker relation, involving exactly these relative quantities.

We begin by recalling that the complete wave function Φ is supported on the product of three semilattices $\mathcal{L}_{\varepsilon_i}^+$, each of which is in turn the union of two semilattices of step four, ${}^{(4)}\mathcal{L}_{\tilde{\varepsilon}_i}$ (where $\tilde{\varepsilon}_i \in \{\varepsilon_i, \varepsilon_i + 2\}$). We then divide the support into eight sectors, corresponding to the eight products of the chosen semilattices of step four, and consider the respective restrictions of Φ to each of them. In each sector, we apply the scattering scheme defined at the beginning of this section. In that scheme, the wave packet $\tilde{\Phi}_-$ is transformed into $\tilde{\Phi}_+$ via the unitary rotation

$$U = \prod_{i=1}^3 e^{2i\phi(\omega_i)}, \quad (4.17)$$

the reflection in the signs of ω_a , and a possible change of global sign.

It seems reasonable to restrict our considerations to states such that *each* of the components $\tilde{\Phi}_-$ corresponding to the sectors introduced above is such that the coefficients A_a , B_a , W_a , Y_a , and X_a , defined in Eqs. (3.19) and (3.22), are finite. This ensures that each of these components has a well-defined associated trajectory (3.18) and a finite dispersion for every finite v_1 . In addition, Eq. (3.23) is satisfied.

Neither the rotation (4.17), nor the reflection in the signs of ω_a , nor the possible change in sign of the wave function will change the expectation value or the dispersion of the operator $\omega_1^2(\omega_2, \omega_3)\omega_a^{-2}$. Therefore, if the coefficients (3.19) and (3.22) are finite also for $\tilde{\Phi}_+$, Eq. (3.23) implies immediately that the following holds

$$\frac{\langle \Delta \ln(\hat{v})_a \rangle_+}{\langle \ln(\hat{v})_a \rangle_+} = \frac{\langle \Delta \ln(\hat{v})_a \rangle_-}{\langle \ln(\hat{v})_a \rangle_-}, \quad (4.18)$$

where $\langle \cdot \rangle_{\pm}$ denote expectation values on $\tilde{\Phi}_{\pm}$, respectively.

To prove that the finiteness of A_a , B_a , W_a , Y_a , and X_a for $\tilde{\Phi}_-$ implies the finiteness of these coefficients for $\tilde{\Phi}_+$, we apply similar methods to those proposed by Kamiński and Pawłowski [37]. Since A_a and W_a are equal for both components, the only ones that require detailed analysis are B_a , Y_a , and X_a . We first recall that

$$B_a = \langle \mathcal{D}_a \rangle, \quad Y_a = \langle \mathcal{D}'_a \rangle, \quad (4.19a)$$

$$X_a - B_a^2 = \langle \Delta \mathcal{D}_a \rangle^2 =: \sigma_{\mathcal{D}_a}^2, \quad (4.19b)$$

where

$$\mathcal{D}_a = -i\alpha|\omega_2 + \omega_3|^{-1/2}(\partial_{\omega_a})|\omega_2 + \omega_3|^{1/2}, \quad (4.20a)$$

$$\mathcal{D}'_a = 2\omega_1(\omega_2, \omega_3)\omega_a^{-1}\mathcal{D}_a\omega_1(\omega_2, \omega_3)\omega_a^{-1}. \quad (4.20b)$$

Knowing the relation between $\tilde{\Phi}_-$ and $\tilde{\Phi}_+$, we can find the relations between their corresponding expectation values (4.19). They are

$$\langle \mathcal{D}_a \rangle_+ = -\langle \mathcal{D}_a \rangle_- - 2\alpha \sum_{i=1}^3 \langle [\partial_{\omega_a} \phi(-\omega_i)] \rangle_-, \quad (4.21a)$$

$$\langle \mathcal{D}'_a \rangle_+ = -\langle \mathcal{D}'_a \rangle_- - 4\alpha \sum_{i=1}^3 \left\langle \frac{\omega_1^2}{\omega_a^2} [\partial_{\omega_a} \phi(-\omega_i)] \right\rangle_-, \quad (4.21b)$$

$$\sigma_{\mathcal{D}_a} \leq \sigma_{\mathcal{D}_a}^- + 2\alpha \sum_{i=1}^3 \langle \Delta [\partial_{\omega_a} \phi(-\omega_i)] \rangle_-. \quad (4.21c)$$

Actually, it is possible to estimate the terms related with $\partial_{\omega_a} \phi(-\omega_i)$ employing that the function $\phi(\omega)$ possesses the following properties [37]:

$$|\partial_{\omega} \phi(\omega)| \leq C_1 |\ln|\omega|| + C_0, \quad (4.22a)$$

$$|\omega \partial_{\omega}^2 \phi(\omega)| \leq C_2, \quad (4.22b)$$

where C_0 , C_1 , and C_2 are (positive) finite constants, which however may depend on the value of the subsemilattice label $\tilde{\varepsilon}_i$ and, in particular, may not have a global bound (in the whole interval of variation of this label).

These inequalities can be next used to relate the terms in Eq. (4.21) with the expectation values and dispersions of the operators $\ln|\omega_i|$. In order to do so, let us first define the multiplicative operators

$$w_a := \omega_1(\omega_2, \omega_3)\omega_a^{-1}, \quad (4.23a)$$

$$\Omega_a^{(n)} := w_a^n \ln|\omega_1(\omega_2, \omega_3)|, \quad (4.23b)$$

$$\Sigma_a^{(n)} := w_a^n \ln|\omega_a|. \quad (4.23c)$$

In the case of relation (4.21a), the last term is bounded as follows

$$\left| \sum_{i=1}^3 \langle [\partial_{\omega_a} \phi(-\omega_i)] \rangle_- \right| \leq C_1 [\langle |\ln|\omega_a|| \rangle_- + \langle |\Omega_a^{(2)}| \rangle_-] + C_0(1 + \langle w_a^2 \rangle), \quad (4.24)$$

whereas for the term in Eq. (4.21b) one has

$$\left| \sum_{i=1}^3 \left\langle \frac{\omega_1^2}{\omega_a^2} [\partial_{\omega_a} \phi(-\omega_i)] \right\rangle_- \right| \leq C_1 [\langle |\Sigma_a^{(2)}| \rangle_- + \langle |\Omega_a^{(4)}| \rangle_-] + C_0 [\langle w_a^2 \rangle + \langle w_a^4 \rangle]. \quad (4.25)$$

Similarly, the sum in (4.21c) satisfies

$$\sum_{i=1}^3 \langle \Delta [\partial_{\omega_a} \phi(-\omega_i)] \rangle_- \leq C_2 [\langle \Delta \ln|\omega_a| \rangle_- + \langle \Delta \Omega_a^{(2)} \rangle_-]. \quad (4.26)$$

Suppose now that in the state $\tilde{\Phi}_-$ the dispersions and expectation values of $\ln|\omega_a|$, $\Omega_a^{(2)}$, and w_a^2 are finite, as well as the expectation values of $\Sigma_a^{(2)}$. This immediately implies the finiteness of the right-hand side of Eqs. (4.24), (4.25), and (4.26) (including that of $\langle |\Omega_a^{(4)}| \rangle_-$). From this and the fact that C_0 , C_1 , $C_2 < \infty$ it is straightforward to check that, if the coefficients B_a , X_a , and Y_a corresponding to $\tilde{\Phi}_-$ are finite, so are the ones corresponding to $\tilde{\Phi}_+$. Therefore, we conclude that Eq. (4.18) is indeed satisfied, as we wanted to prove.

It is worth noticing that, in the previous discussion, the roles of $\tilde{\Phi}_+$ and $\tilde{\Phi}_-$ can be interchanged, so that one can instead impose mild conditions of the type explained above on $\tilde{\Phi}_+$ and ensure then a good behavior for the relative dispersions corresponding to $\tilde{\Phi}_-$.

Finally, in Appendix A we show that our result (4.18) about the relative dispersions can actually be extended to the case in which one takes into consideration not just one isolated sector, but the whole ensemble of the eight sectors in which the LQC physical states admit a WDW limit. In this way, we arrive at the following conclusion. Consider a physical state described by the wave function Φ supported on the product of semilattices $\mathcal{L}_{\varepsilon_1}^+ \times \mathcal{L}_{\varepsilon_2}^+ \times \mathcal{L}_{\varepsilon_3}^+$. Suppose that the restriction of Φ to the product of subsemilattices ${}^{(4)}\mathcal{L}_{\tilde{\varepsilon}_1}^+ \times {}^{(4)}\mathcal{L}_{\tilde{\varepsilon}_2}^+ \times {}^{(4)}\mathcal{L}_{\tilde{\varepsilon}_3}^+$ possesses a WDW limit such that the component $\tilde{\Phi}_{\pm}$ moving forward/backward in time has finite expectation values and dispersions for the operators

$$\ln(\hat{v}_a)_{v_1}, \quad \ln|\omega_a|, \quad \Omega_a^{(2)}, \quad w_a^2. \quad (4.27)$$

Suppose also that this state has finite expectation values for the operators

$$\Sigma_a^{(2)}. \quad (4.28)$$

Then

- (i) the corresponding component $\tilde{\Phi}_{\mp}$ moving backward/forward in time has also finite expectation values and dispersions with respect to the operators (4.27), as well as finite expectation values for the operators (4.28), and
- (ii) relation (4.18) holds for the ensemble of the WDW limits corresponding to all of the eight sectors defined by the restrictions to the different subsemilattices, constructed to reflect the relevant features of a complete LQC state (see Appendix A for the discussion).

V. DESCRIPTION ON v -SECTIONS: UNITARY EVOLUTION

In the case of the WDW quantization, we introduced in Sec. III C the notion of evolution by means of a family of observables which are related via unitary transformations. In this section we will analyze the possibility of performing an analogous construction in the LQC model. First, in Sec. VA, we will establish the relation between the physical Hilbert space and an appropriate space of “initial” data defined on a single slice $v_1 = \text{const}$. That relation will be used in Sec. VB to construct a direct analog of the family (3.14), which however fails to admit a unitary relation. In Sec. VC, certain modification of the construction will allow us to overcome this problem, although at the price of loosing a neat physical interpretation of the selected observables, which is recovered only in the large v_1 limit. The modified observables are finally used in Sec. VD to extract physical predictions, which are presented in Sec. VE.

A. Time slices and associated Hilbert spaces

Let us start with the general form of the wave function that represents the physical state, given by Eq. (2.12). In analogy with the procedure explained in Sec. III C, we choose as the internal time the variable v_1 and define the “initial data” functions on each slice $v_1 = \text{const}$ in the following way

$$\Phi_{v_1}(v_2, v_3) = \int_{\mathbb{R}^2} d\omega_2 d\omega_3 \tilde{\Phi}_{v_1}(\omega_2, \omega_3) e^{\varepsilon_2}_{\omega_2}(v_2) e^{\varepsilon_3}_{\omega_3}(v_3), \quad (5.1)$$

where the spectral profiles $\tilde{\Phi}_{v_1}(\omega_2, \omega_3)$ of $\Phi_{v_1}(v_2, v_3)$ belong to the slice Hilbert spaces

$$\mathcal{H}_{v_1} := L^2(\mathbb{R}^2, |\omega_2 + \omega_3| |e^{\varepsilon_1}_{\omega_1}(v_1)|^{-2} d\omega_2 d\omega_3), \quad (5.2)$$

and are defined by the transformation $P_{v_1}: \mathcal{H}_{\varepsilon}^{\text{Phys}} \rightarrow \mathcal{H}_{v_1}$

$$\tilde{\Phi}_{v_1}(\omega_2, \omega_3) := P_{v_1} \tilde{\Phi}(\omega_2, \omega_3) := \tilde{\Phi}(\omega_2, \omega_3) e^{\varepsilon_1}_{\omega_1}(v_1). \quad (5.3)$$

On any slice $v_1 = \text{const}$, $e^{\varepsilon_1}_{\omega_1}(v_1)$ provides just a function of ω_1 which turns out to vanish in a set of zero measure [see Eq. (45) in Ref. [9] for the details]. Therefore, the map P_{v_1} is unitary. This property, together with the fact that both $e^{\varepsilon_2}_{\omega_2}(v_2)$ and $e^{\varepsilon_3}_{\omega_3}(v_3)$ form bases of their corresponding kinematical spaces $\mathcal{H}_{\varepsilon_a}^+$, allows us to determine $\tilde{\Phi}(\omega_2, \omega_3)$ from $\Phi_{v_1}(v_2, v_3)$ (up to a zero measure set). As a consequence, the projection on each v_1 -slice contains the same information as the entire physical solution. However, one cannot write the inner product of (5.2) as an integral of $\Phi_{v_1}(v_2, v_3)$ with well-defined Lebesgue measure. Owing to the dependence of $|e^{\varepsilon_1}_{\omega_1}(v_1)|$ in ω_2 and ω_3 , the inner product of $\mathcal{H}_{v_1}$ is nonlocal when expressed in terms of v_2 and v_3 .

The unitary transformation P_{v_1} allows us to define a map between initial data spaces. Each state on the physical Hilbert space $\mathcal{H}_{\varepsilon}^{\text{Phys}}$ is associated, through P_{v_1} , with a sequence of elements of the slice spaces $\mathcal{H}_{v_1}$. Each sequence consists in the chain of “evolution steps” enumerated by $v_1 \in \mathcal{L}_{\varepsilon_1}^+$. However, the corresponding evolution is not unitary, because under the identification of different slices, initial data belonging to one of the spaces $\mathcal{H}_{v_1}$ will in general not belong to the others, since $|e^{\varepsilon_1}_{\omega_1}(v_1)|$ depends on v_1 . In the next subsection we will try to provide a more sophisticated notion of evolution free of this problem by building a set of observables analogous to the family (3.14) that we constructed for the WDW model.

B. v_1 -observables

Once we have introduced the Hilbert spaces (5.2), and the transformations between them and $\mathcal{H}_{\varepsilon}^{\text{Phys}}$, we can follow the construction of relational observables made in Sec. III C, starting from the kinematical observables $\ln(\hat{v}_a)$ ($a = 2, 3$), which also act as multiplication operators here. However, unlike the WDW eigenfunctions $e_{\omega_1}(v_1)$, the eigenfunctions $e^{\varepsilon_1}_{\omega_1}(v_1)$ have a phase which is v_1 -independent separately on each of the subsemilattices $(4)\mathcal{L}_{\varepsilon_1}^+$ and $(4)\mathcal{L}_{\varepsilon_1+2}^+$, with a global phase shift of $\pi/2$ between them (see Sec. II C). Therefore the transformation between $\mathcal{H}_{v_1}$ and $\mathcal{H}'$ analogous to (3.12) essentially removes all the information from the state. As a consequence, the observables constructed in this way do not carry physically interesting information.

As an alternative, one may adopt a more naive approach, which consists in considering the operators $\ln(\hat{v}_a)$ just as multiplication operators acting on the elements of $\mathcal{H}_{v_1}$ in the v_a -representation:

$$[\ln(\hat{v}_a)\Phi_{v_1}](v_2, v_3) = \ln(v_a)\Phi_{v_1}(v_2, v_3). \quad (5.4)$$

We can rewrite the action of these operators in terms of the variables ω_a and represent them as operators on the physical Hilbert space $\mathcal{H}_{\varepsilon}^{\text{Phys}}$ using Eq. (5.3). In particular, $\ln(\hat{v}_2)_{v_1}$ acts on $\tilde{\Phi} \in \mathcal{S}(\mathbb{R}^2) \subset \mathcal{H}_{\varepsilon}^{\text{Phys}}$ as follows:

$$[\ln(\hat{v}_2)_{v_1} \tilde{\Phi}](\omega_2, \omega_3) = \frac{1}{e^{\varepsilon_1}_{\omega_1}(v_1)} \int d\omega'_2 \langle e^{\varepsilon_2}_{\omega'_2} | \ln(\hat{v}_2) e^{\varepsilon_2}_{\omega'_2} \rangle_{\mathcal{H}_{\varepsilon_2}^+} \times e^{\varepsilon_1}_{\omega_1(\omega'_2, \omega_3)}(v_1) \tilde{\Phi}(\omega'_2, \omega_3), \quad (5.5)$$

whereas the action of $\ln(\hat{v}_3)$ is the same with the subindex 2 replaced with 3. This implies immediately that two operators at different times, e.g. $\ln(\hat{v}_a)_{v_1}: \mathcal{H}_{\varepsilon}^{\text{Phys}} \rightarrow \mathcal{H}_{\varepsilon}^{\text{Phys}}$ and $\ln(\hat{v}_a)_{v_1^*}: \mathcal{H}_{\varepsilon}^{\text{Phys}} \rightarrow \mathcal{H}_{\varepsilon}^{\text{Phys}}$, are related via the transformation

$$\hat{Q}_{v_1, v_1^*}: \mathcal{H}_{\tilde{\varepsilon}}^{\text{Phys}} \rightarrow \mathcal{H}_{\tilde{\varepsilon}}^{\text{Phys}},$$

$$[\hat{Q}_{v_1, v_1^*} \tilde{\Phi}](\omega_2, \omega_3) = \left[\frac{e_{\omega_1}^{\varepsilon_1}(v_1)}{e_{\omega_1}^{\varepsilon_1}(v_1^*)} \right] \tilde{\Phi}(\omega_2, \omega_3), \quad (5.6)$$

so that

$$\ln(\hat{v}_a)_{v_1^*} = \hat{Q}_{v_1, v_1^*} \ln(\hat{v}_a)_{v_1} \hat{Q}_{v_1^*, v_1}. \quad (5.7)$$

Since the amplitude $|e_{\omega_1}^{\varepsilon_1}(v_1)|$ changes significantly both when ω_1 or v_1 varies, the operators $\hat{Q}_{v_1, v_1^*}$ are not unitary. Hence, the family of observables defined here *fails to be unitarily related*.

In order to attain a notion of nontrivial unitary evolution in v_1 , we propose in the next subsection a particular construction which exploits the asymptotic properties of $e_{\omega_1}^{\varepsilon_1}(v_1)$ and their relation with their WDW analogs $\underline{e}_{\omega_1}(v_1)$.

C. v_1 -observables on components

The success of the construction of Sec. III C to provide a nontrivial evolution picture for the WDW model rests in the form of the eigenfunctions $\underline{e}_{\omega_1}(v_1)$ of the operator $\hat{\Theta}_1$, which are essentially rotating complex functions. In LQC, the analogous eigenfunctions $e_{\omega_1}^{\varepsilon_1}(v_1)$ oscillate rather than rotate. Furthermore, on each of the subsemilattices $^{(4)}\mathcal{L}_{\varepsilon_1}^+$ and $^{(4)}\mathcal{L}_{\varepsilon_1+2}^+$, these elements converge to a combination of incoming and outgoing WDW eigenfunctions, both contributing with equal amplitude. In this sense, each eigenfunction $e_{\omega_1}^{\varepsilon_1}(v_1)$ of $\hat{\Theta}_1$ can be interpreted as a standing wave, which contains both components moving forward and backward in time. This interpretation is supported by the studies of the classical effective dynamics of the system performed in Ref. [20], where a bounce in the internal time v_1 is observed.

These considerations suggest that, rather than trying to construct the analogs of the WDW observables $\ln(\hat{v}_a)_{v_1}$, one should build instead two separate families $\ln(\hat{v}_a)_{v_1}^{\pm}$, each corresponding to one of the two commented components of the wave function. With respect to the procedure specified in Sec. III C, this can be viewed as a specific choice of *two* (instead of one) auxiliary Hilbert spaces: $\mathcal{H}^{I+}$ and $\mathcal{H}^{I-}$.

In order to define the decomposition in a precise form, we first introduce the following transformation of the eigenfunctions of $\hat{\Theta}_1$, defined in the distributional sense on each of the subsemilattices $^{(4)}\mathcal{L}_{\varepsilon_1}^+$ and $^{(4)}\mathcal{L}_{\varepsilon_1+2}^+$ separately:

$$e_{\omega_1}^{\varepsilon_1} \rightarrow e_{\omega_1}^{\tilde{\varepsilon}_1 s} = \mathcal{F}^{-1} \theta[-s(b_1 - \pi/2)] \mathcal{F} e_{\omega_1}^{\varepsilon_1}, \quad (5.8)$$

where $s \in \{+, -\}$, $\tilde{\varepsilon}_1 \in \{\varepsilon_1, \varepsilon_1 + 2\}$, θ is a Heaviside step function, b_1 is the momentum conjugate to v_1 [see Eqs. (3.24) and (3.25)], and $\mathcal{F}$ is a discrete Fourier transform analogous to the one defined for isotropic systems in Refs. [12, 15]:

$$[\mathcal{F}f](b_1) = \sum_{v_1 \in ^{(4)}\mathcal{L}_{\tilde{\varepsilon}_1}^+} f(v_1) v_1^{-1/2} e^{-(i/2)v_1 b_1}, \quad b_1 \in [0, \pi]. \quad (5.9)$$

The introduction of the rescaling by $v_1^{-1/2}$ in this transformation is needed to develop the analysis of the evolution in terms of b_1 that we carry out in Sec. VI. Therefore, we use the same Fourier transform here.

The transformation (5.8) essentially extracts in each subsemilattice the components (labeled by $+$ and $-$) of $e_{\omega_1}^{\tilde{\varepsilon}_1}$ that, respectively, converge, in the large v_1 limit, to the WDW analogs $\underline{e}_{-\omega_1}$ and $\underline{e}_{\omega_1}$, which move backward and forward in time.

The functions $e_{\omega_1}^{\tilde{\varepsilon}_1 s}$ sum up to the original eigenfunctions $e_{\omega_1}^{\tilde{\varepsilon}_1}$, therefore one can split any wave function Φ_{v_1} , defined in Eq. (5.1), into rotating components $\Phi_{v_1}^s$ simply by replacing the eigenfunctions $e_{\omega_1}^{\varepsilon_1}$ in Eq. (5.3) with $e_{\omega_1}^{\varepsilon_1 s}$ [39]. However, the Hilbert spaces $\mathcal{H}_{v_1}^s \supset \Phi_{v_1}^s$, which are the analogs of $\mathcal{H}_{v_1}$ [in the sense of the definition (5.2)], still have different inner products for different v_1 , since $|e_{\omega_1}^{\varepsilon_1 s}|$ depends on v_1 . Thus, to “synchronize” the norms we include one more step in the splitting, namely, the normalization of $e_{\omega_1}^{\varepsilon_1 s}$ into pure phases, and introduce the corresponding auxiliary Hilbert spaces $\mathcal{H}^{Is}$, analogs of (3.11). The final splitting $\mathcal{H}_{\tilde{\varepsilon}}^{\text{Phys}} \rightarrow \mathcal{H}^{Is}$ is thus defined (on the bases of the Hilbert spaces) as follows

$$e_{\omega_1}^{\varepsilon_1} \mapsto e_{\omega_1}^{Is} := |\omega_2 + \omega_3|^{1/2} \frac{e_{\omega_1}^{\varepsilon_1 s}}{|e_{\omega_1}^{\varepsilon_1 s}|}. \quad (5.10)$$

The implementation of this splitting allows us to define the projection $\hat{R}_{v_1}^s$ of the physical states onto rotating components:

$$\hat{R}_{v_1}^s: \mathcal{H}_{\tilde{\varepsilon}}^{\text{Phys}} \rightarrow \mathcal{H}^{Is}, \quad \mathcal{H}^{Is} = L^2(\mathbb{R}^2, d\omega_2 d\omega_3),$$

$$[\hat{R}_{v_1}^s \tilde{\Phi}](\omega_2, \omega_3) = \tilde{\chi}_{v_1}^s(\omega_2, \omega_3) := \tilde{\Phi}(\omega_2, \omega_3) e_{\omega_1}^{Is}(v_1). \quad (5.11)$$

Using these projections we can finally define two families of observables: $\ln(\hat{v}_a)_{v_1}^+: \mathcal{H}_{\tilde{\varepsilon}}^{\text{Phys}} \rightarrow \mathcal{H}_{\tilde{\varepsilon}}^{\text{Phys}}$ and $\ln(\hat{v}_a)_{v_1}^-: \mathcal{H}_{\tilde{\varepsilon}}^{\text{Phys}} \rightarrow \mathcal{H}_{\tilde{\varepsilon}}^{\text{Phys}}$, starting from the kinematical operators $\ln(\hat{v}_a)$. Their action on $\mathcal{H}_{\tilde{\varepsilon}}^{\text{Phys}}$ is analogous to Eq. (5.5),

$$[\ln(\hat{v}_a)_{v_1}^s \tilde{\Phi}](\omega_2, \omega_3) = \frac{1}{e_{\omega_1}^{Is}(v_1)} \int d\omega'_2 \langle e_{\omega_2}^{\varepsilon_2} | \ln(\hat{v}_a) e_{\omega'_2}^{\varepsilon_2} \rangle_{\mathcal{H}_{\varepsilon_2}^+} \\ \times e_{\omega_1(\omega'_2, \omega_3)}^{Is}(v_1) \tilde{\Phi}(\omega'_2, \omega_3). \quad (5.12)$$

Within each particular family labeled by a and s , two observables evaluated at different times v_1 and v_1^* are related via the operators

$$\begin{aligned} \hat{Q}_{v_1, v_1^*}^s: \mathcal{H}_{\varepsilon}^{\text{Phys}} &\rightarrow \mathcal{H}_{\varepsilon}^{\text{Phys}}, \\ [\hat{Q}_{v_1, v_1^*}^s \tilde{\Phi}](\omega_2, \omega_3) &= \frac{e^{i\varepsilon_1^s(v_1)}}{e^{i\varepsilon_1^s(v_1^*)}} \tilde{\Phi}(\omega_2, \omega_3), \end{aligned} \quad (5.13)$$

in the following way

$$\ln(\hat{v}_a)_{v_1^*}^s = \hat{Q}_{v_1, v_1^*}^s \ln(\hat{v}_a)_{v_1}^s \hat{Q}_{v_1^*, v_1}^s. \quad (5.14)$$

Since, by definition (5.10), $|e_{\omega_1^s}^{i\varepsilon_1^s}(v_1)| = |\omega_2 + \omega_3|^{1/2}$ for all $v_1 \in \mathcal{L}_{\varepsilon_1}^+$, the operators $\hat{Q}_{v_1, v_1^*}^s$ are unitary and, therefore, within each family the considered observables are *unitarily related*. We can again extend the set formed by these families, adding the operators $\hat{\Theta}_a|_{v_1} := \hat{\Theta}_a$, to obtain a complete set of observables.

Thus, the operators defined in Eq. (5.12) provide a correct notion of unitary evolution. However, this comes at a price. Owing to the normalization (5.10), the observables no longer have a precise physical interpretation. Such an interpretation can be recovered only asymptotically for large v_1 , where the rotating components $e_{\omega_1^s}^{i\varepsilon_1^s}$ approach their WDW analogs (see Sec. II C) and $|e_{\omega_1^s}^{i\varepsilon_1^s}|$ converges to an ω_a -independent function [see Eq. (3.4)]. As a consequence, one can interpret the operators $\ln(\hat{v}_a)_{v_1}^s$ only approximately as evaluating $\ln(v_a)$ at the given value of v_1 on the component that is moving forward (for negative sign) or backward (for positive sign) in time. The approximation improves as v_1 increases; however, for v_1 of the order of ω_1 or smaller (where the effective theory predicts a bounce in v_1) all the precision is lost. An illustrative argument which shows the “unreliability” of the interpretation of $\ln(\hat{v}_a)_{v_1}^s$ in such regime is presented in Sec. V E, where we discuss the application of the construction introduced here to analyze the dynamics of physical states which are semiclassical at late times.

D. Numerical aspects of the analysis

In this subsection we describe the numerical methods used to analyze the dynamics of the model. The reader that is not interested in these numerical aspects can safely skip this part and go to Sec. V E, where the results are presented.

We focus our discussion on physical states that are semiclassical at late times; more precisely, on Gaussian states (4.14) peaked around large (ω_2^*, ω_3^*) [whose late time trajectory is determined by (β^2, β^3) via Eq. (4.16)]. The wave functions corresponding to such states, given by the integral (2.12), are next evaluated applying the trapezoid method in the domain $\omega_a \in [\omega_a^* - 5\sigma_a, \omega_a^* + 5\sigma_a]$. $\tilde{\Phi}(\omega_2, \omega_3)$ has been probed within the uniform grid defined by the split of the domain into at least $2\omega_a^*$ subintervals in each direction.

To find the expectation values of $\ln(v_a)_{v_1}^s$ we have used the expression of the elements $\tilde{\chi}_{v_1}^s(\omega_2, \omega_3)$ of $\mathcal{H}^{ls}$ as functions of v_a ,

$$\chi_{v_1}^s(v_2, v_3) = \int_{\mathbb{R}^2} d\omega_2 d\omega_3 \tilde{\chi}_{v_1}^s(\omega_2, \omega_3) e_{\omega_2}^{\varepsilon_2}(v_2) e_{\omega_3}^{\varepsilon_3}(v_3). \quad (5.15)$$

Since $e_{\omega_a}^{\varepsilon_a}(v_a)$ form orthonormal bases on their respective kinematical spaces $\mathcal{H}_{\varepsilon_a}^+$, the physical inner product (2.14) on $\mathcal{H}^{ls}$ takes a very simple form in the v_a -representation

$$\langle \chi_{v_1}^s | \chi_{v_1'}^s \rangle = \sum_{\mathcal{L}_{\varepsilon_2}^+ \times \mathcal{L}_{\varepsilon_3}^+} \tilde{\chi}_{v_1}^s(v_2, v_3) \chi_{v_1'}^s(v_2, v_3). \quad (5.16)$$

Furthermore, on $\chi_{v_1}^s(v_2, v_3)$ the observables $\ln(\hat{v}_a)_{v_1}^s$ act just as multiplication operators

$$[\ln(\hat{v}_a)_{v_1}^s \chi_{v_1}^s](v_2, v_3) = \ln(v_a) \chi_{v_1}^s(v_2, v_3). \quad (5.17)$$

Hence, their expectation values on the state Φ are

$$\langle \Phi | \ln(\hat{v}_a)_{v_1}^s | \Phi \rangle = \|\chi_{v_1}^s\|^{-2} \sum_{\mathcal{L}_{\varepsilon_2}^+ \times \mathcal{L}_{\varepsilon_3}^+} \ln(v_a) |\chi_{v_1}^s(v_2, v_3)|^2, \quad (5.18)$$

where $\chi_{v_1}^s$ is related to Φ via Eq. (5.11).

The dispersions corresponding to $\ln(\hat{v}_a)_{v_1}^s$ are given by the standard formula

$$\langle \Delta \ln(\hat{v}_a)_{v_1}^s \rangle^2 = \langle (\ln(\hat{v}_a)_{v_1}^s)^2 \rangle - \langle \ln(\hat{v}_a)_{v_1}^s \rangle^2, \quad (5.19)$$

where the expectation values of $[\ln(\hat{v}_a)_{v_1}^s]^2$ are evaluated as we have explained for $\langle \Phi | \ln(\hat{v}_a)_{v_1}^s | \Phi \rangle$.

In the numerical simulations, in order to calculate these expectation values we have first evaluated the components $e_{\omega_1^s}^{i\varepsilon_1^s}$ given in Eq. (5.8) with the use of the Fast Fourier Transform (FFT) algorithm, and then the normalized components $e_{\omega_1^s}^{i\varepsilon_1^s}$ according to Eq. (5.10). After calculating the auxiliary profiles $\tilde{\chi}_{v_1}^s(\omega_2, \omega_3)$, defined by Eq. (5.11), we have evaluated their wave functions $\chi_{v_1}^s(v_2, v_3)$ via direct integration of Eq. (5.15), in a similar way as explained for the evaluation of $\Phi(\vec{v})$. Next, we have found the expectation values computing the summation in Eq. (5.18). The domains of v_a have been restricted to $\mathcal{L}_{\varepsilon_a}^+ \cap [0, 4\omega_a^*]$, and the values of v_1 to the set $\mathcal{L}_{\varepsilon_1}^+ \cap [0, 2 \times 10^5]$. Finally, we have performed simulations for various values of $\tilde{\varepsilon}$ and for ω_a^* ranging from 2.5×10^2 to 10^3 .

E. Results and discussion

In Fig. 2 we show two examples of the results of our numerical study. In all cases, the analysis reveals that

- (i) Inasmuch as the expectation values (5.18) are concerned, the states remain *sharply peaked for all* values of v_1 . This applies to *both* components moving forward and backward in time.
- (ii) For $v_1 \gg \omega_a^*$, the expectation values *follow the classical trajectories*, whereas, when the universe approaches the classical singularity, the discrete geometry effects induce repulsive forces which cause

bounces in both v_2 and v_3 at the values predicted by the effective dynamics.

These results prove the robustness of the big bounce scenario of LQC, extending its validity to another system: the vacuum Bianchi I cosmologies. They confirm as well the ability of the effective dynamics to predict correct results with errors much lower than the spread of the wave function.

Nonetheless, there is one aspect of the results which requires special comments. As one can see in Fig. 2, while for large v_1 the expectation values of the observables $\ln(\hat{v}_a)_{v_1}^s$ follow the classical trajectories (with decreasing precision for decreasing v_1), for $v_1 \lesssim 0.2\omega_1(\omega_2^*, \omega_3^*)$ the expectation values of both families “freeze” at the same trajectory of constant v_2 and v_3 . However this behavior does not correspond to that of $\ln(v_a)$ at given v_1 in any physical way, since $\ln(\hat{v}_a)_{v_1}^s$ no longer approximates it (for each a) in that region.

To illustrate this fact, let us consider a slight modification of the proposed scheme for the construction of observables. So far, we have used v_1 as an emergent time; however, owing to the symmetry of the system, any of the variables v_i can play this role. Therefore, for a given physical state which is semiclassical at late times, we can consider, e.g., the two following constructions: $\ln(\hat{v}_a)_{v_1}^s$ and $\ln(\hat{v}_{a'})_{v_2}^s$, where $a' = 1, 3$, and compare the corresponding expectation values. Such comparison is presented in Fig. 3. Outside the regions where the effective dynamics predicts bounces, the trajectories formed by the two considered families agree. However, once the value of the emergent time corresponding to each of the families drops below that of the point where the effective bounce occurs,

FIG. 3 (color online). Comparison of the expectation values of the two families of observables $\ln(\hat{v}_2)_{v_1}^+$ (blue) and $\ln(\hat{v}_1)_{v_2}^+$ (red), corresponding to two different choices of emergent time, calculated on the state considered in Fig. 2(a).

we observe significant discrepancies in the resulting trajectories. Indeed, while one family shows a bounce, the other predicts the freezing of the trajectory, and vice versa. This implies that in such regions the trajectories *cannot be interpreted* as corresponding to the value of $\ln(v_i)$ at given emergent time in any (even approximate) sense. The applicability of the observables associated with v_i -slices and with v_i as an emergent time is thus limited from a physical viewpoint.

In order to obtain a more reliable description, with a valid physical interpretation in all the interesting regions, we have to use a different construction of observables. Such construction will be presented in the next section,

FIG. 2 (color online). For Gaussian states [with profile (4.14)], the expectation values and dispersions of the observables $\ln(\hat{v}_a)_{v_1}^+$ and $\ln(\hat{v}_a)_{v_1}^-$ [corresponding to epochs when the wave packet is moving forward (green error bars) and backward (red error bars) in time, respectively] are compared with classical (pink lines) and effective (blue dotted line) trajectories. The states are peaked at $\omega_2^* = \omega_3^* = 10^3$ with the relative dispersions $\Delta\Theta_2/\Theta_2 = \Delta\Theta_3/\Theta_3 = 0.05$. The phases are, respectively, $\beta^2 = \beta^3 = 0$ for (a), and $\beta^2 = \beta^3 = 0.1$ for (b). The expectation values follow the effective trajectory till the point of bounce in v_1 , where the dynamics “freezes”. On the other hand away from the bounce the quantum trajectory approaches the classical ones. In particular, in (a) the trajectories before and after the bounce coincide on the plane v_1 - v_2 .

where as emergent time, instead of v_1 , we choose its conjugate momentum b_1 .

VI. UNITARY EVOLUTION ON b -SECTIONS

One of the main reasons why the analog of the WDW observables defined on v_1 -slices fail to provide a unitary evolution in the loop quantization is the fact that the variable chosen as emergent time does not possess all the ideal properties of this kind of time. Indeed, an analysis of the dynamics at the effective level [20] and of the properties of the eigenfunctions (see Sec. IIC) shows that v_1 is not monotonous in the proper time (see also Appendix B). This forced us to define two families of operators corresponding to epochs when the universe is, respectively, contracting and expanding in v_1 . Such a splitting can be avoided if we identify a phase space variable which changes monotonously with time. Here again the effective dynamics comes to the aid, showing that any canonically conjugate momentum b_i of v_i possesses the desired property, so that it may be a promising candidate for an emergent time in the genuine quantum theory.

In this section we explore this possibility by replacing the configuration variable v_1 with its momentum b_1 and representing $\mathcal{H}_{\tilde{e}}^{\text{Phy}}$ by Hilbert spaces of data on $b_1 = \text{const}$ slices (in analogy with the v_1 -slices discussed in Sec. VA). This step is described in Sec. VIA. We then introduce in Sec. VIB the observables corresponding to $\ln(v_i)$ at a given b_1 . The constructed family of operators is used in Sec. VIC to carry out a numerical analysis of physical states, whose results are presented in Sec. VID.

A. b -representation

Let us start by choosing at the classical level the momentum b_1 conjugate to v_1 which is defined through Eqs. (3.24) and (3.25). In our quantization, the transformation between the “position” and “momentum” representations is given by the formula

$$[\mathcal{F}\psi](b_i) = \sum_{\mathcal{L}_{e_i}^+} \psi(v_i) v_i^{-1/2} e^{-(i/2)v_i b_i}. \quad (6.1)$$

As commented in Sec. VC, we have introduced an additional rescaling by $v_i^{-1/2}$ in comparison with Eq. (3.26). The reason for that is twofold: the rescaling guarantees a proper convergence in order to perform the transformation numerically and, in addition, ensures a more convenient behavior of the transformed eigenfunctions (see Sec. VIC). Under this transformation, the kinematical operators which enter the Hamiltonian constraint and the observables change as follows

$$\begin{aligned} \hat{v}_i &\rightarrow 2i\partial_{b_i}, \\ \hat{v}_1^{1/2}(\hat{\mathcal{N}}_{2\bar{\mu}_i} - \hat{\mathcal{N}}_{-2\bar{\mu}_i})\hat{v}_1^{-1/2} &\rightarrow 2i\sin(\hat{b}_i), \end{aligned} \quad (6.2)$$

where $\hat{b}_i$ acts in the new representation by multiplication.

Since, in order to construct the physical state, we restrict the analysis to one superselection sector, with functions supported on $\mathcal{L}_{e_i}^+$, the same restriction applies to the transformation (6.1). In this case, the domain of b_i can be taken as the unit circle $b_i \in S^1$. Moreover, to further adapt the transformation to our specific system, let us note the following:

- (i) The restrictions of the eigenfunctions of $\hat{\Theta}_i$ (supported on $\mathcal{L}_{e_i}^+$) to the subsemilattices $^{(4)}\mathcal{L}_{e_i}^+$ and $^{(4)}\mathcal{L}_{e_i+2}^+$ are eigenfunctions of $\hat{\Theta}_i^2$, which differs from the evolution operator of the isotropic system just by a compact operator (see Ref. [9] and Sec. IIC).
- (ii) Since, e.g., any $v_1 = \text{const}$ section contains all the information about a physical state, in particular, the restriction of a physical state to one of the subsemilattices for v_1 uniquely determines the other.
- (iii) In the isotropic model and within the context of solvable LQC (sLQC) [12] a similar transformation allows one to select the domain of the corresponding momentum b as $[0, \pi)$. Furthermore, the sLQC analog of $\hat{\Theta}_i^2$ is proportional to $[\sin(b)\partial_b]^2$. This in turn allows one to write the constraint as a Klein-Gordon equation.

This last point indicates that it is convenient to apply the transformation (6.1) to functions supported on $^{(4)}\mathcal{L}_{e_i}^+$ and $^{(4)}\mathcal{L}_{e_i+2}^+$ independently. The domain of b_i consists then of two copies of the circle with radius one half (i.e., the periodicity of b_i is π in each copy). As a consequence, one can define the transformation $\mathcal{F}$ such that

$$[\mathcal{F}_1\psi](b_i) = \sum_{v_i \in ^{(4)}\mathcal{L}_{e_i}^+} \psi(v_i) v_i^{-1/2} e^{-(i/2)v_i b_i}, \quad (6.3)$$

and, analogously, the transformation $\mathcal{F}_2$ by choosing the summation over $^{(4)}\mathcal{L}_{e_i+2}^+$ instead of $^{(4)}\mathcal{L}_{e_i}^+$.

If we transform the eigenfunctions of $\hat{\Theta}_1$, we can define a “mixed” representation of physical states

$$\begin{aligned} \Phi(b_1, v_2, v_3) &= \int_{\mathbb{R}^2} d\omega_2 d\omega_3 \tilde{\Phi}(\omega_2, \omega_3) \tilde{e}_{\omega_1}^{e_1}(b_1) e_{\omega_2}^{e_2}(v_2) \\ &\quad \times e_{\omega_3}^{e_3}(v_3), \end{aligned} \quad (6.4)$$

where $\tilde{e}_{\omega_1}^{e_1}(b_1)$ is

$$\tilde{e}_{\omega_1}^{e_1}(b_1) = \begin{cases} [\mathcal{F}_1 e_{\omega_1}^{e_1}](b_1), & b_1 \in [0, \pi) \\ [\mathcal{F}_2 e_{\omega_1}^{e_1}](b_1 - \pi), & b_1 \in [\pi, 2\pi). \end{cases} \quad (6.5)$$

As discussed above, we restrict our considerations, for example, to the domain of b_1 which corresponds to the first of these cases: $b_1 \in [0, \pi)$. Within this domain, one can now apply the analog of the constructions presented in Sec. III and V. In doing so, we introduce the counterpart of the spaces $\mathcal{H}_{v_1}$ [given in Eq. (5.2)], which are defined on surfaces of constant b_1 ,

$$\mathcal{H}_{b_1} := L^2(\mathbb{R}^2, |\omega_2 + \omega_3| |\tilde{e}_{\omega_1}^{\varepsilon_1}(b_1)|^{-2} d\omega_2 d\omega_3), \quad (6.6)$$

and the transformation of the physical states into elements in these spaces

$$\hat{P}_{b_1}: \mathcal{H}_{\tilde{e}}^{\text{Phys}} \rightarrow \mathcal{H}_{b_1}, \quad (6.7a)$$

$$[\hat{P}_{b_1} \tilde{\Phi}](\omega_2, \omega_3) = \tilde{\Phi}_{b_1}(\omega_2, \omega_3) := \tilde{e}_{\omega_1}^{\varepsilon_1}(b_1) \tilde{\Phi}(\omega_2, \omega_3). \quad (6.7b)$$

Each function $\tilde{\Phi}_{b_1}$ at any given slice $b_1 = \text{const}$ determines the physical state uniquely, thus it can be understood as the initial data at that slice. Therefore, one may develop a notion of evolution in b_1 using the corresponding map between initial data spaces. It is worth noticing, nonetheless, that, unlike in sLQC (and with the chosen factor ordering), the Hamiltonian constraint (2.5) in a b_i -representation cannot be expressed as a differential equation of finite order.

B. Observables associated with b -slices

With the spaces of initial data at constant b_1 at our disposal, we can now define the observables $\ln(v_i)_{b_1}$. For $i = 2, 3$ the construction is completely parallel to that presented in Sec. VB; however, it suffers from a similar problem of lack of a unitary relation between the operators in each family of observables. Here, nevertheless, the problem is much less severe. Indeed, the functions $\tilde{e}_{\omega_1}^{\varepsilon_1}(b_1)$ are (except possibly for small ω_1) rotating functions that never vanish (see Sec. VIC). This property has a qualitative analytical explanation. Actually, the operator $\mathcal{F}_1(\hat{\Theta}_1^2)$ is, up to a compact correction, equal to $-[12\pi\gamma G \sin(b_1) \partial_{b_1}]^2$, whose eigenspaces are spanned by basis elements of the form $N e^{\pm i k x(b_1)}$, with $x(b_1) := \ln[\tan(b_1/2)]$ and where $N = N(k)$ is a normalization factor. Furthermore, once we restrict the space to functions supported on $v_1 > 0$ (as happens to be the case in our model), the eigenfunctions reduce just to purely rotating functions [with vanishing contribution of one of the two phases $\pm i k x(b_1)$]. These eigenfunctions will differ from those of the actual operator $\mathcal{F}_1(\hat{\Theta}_1^2)$ just by small corrections whose (kinematical) norm decreases with ω_1 .

As a consequence, we do not need to split the eigenfunctions into rotating components in order to form a family of unitarily related observables. The following parallel of the transformation (5.10):

$$\tilde{e}_{\omega_1}^{\varepsilon_1}(b) \rightarrow \tilde{e}_{\omega_1}^{\varepsilon_1}(b) = |\omega_2 + \omega_3|^{1/2} \frac{\tilde{e}_{\omega_1}^{\varepsilon_1}(b)}{|\tilde{e}_{\omega_1}^{\varepsilon_1}(b)|} \quad (6.8)$$

is sufficient to build analogs $\hat{R}_{b_1}$ of the operators $\hat{R}_{v_1}^s$,

$$\hat{R}_{b_1}: \mathcal{H}_{\tilde{e}}^{\text{Phys}} \rightarrow \mathcal{H}'_{b_1} := L^2(\mathbb{R}^2, d\omega_2 d\omega_3), \quad (6.9a)$$

$$[\hat{R}_{b_1} \tilde{\Phi}](\omega_2, \omega_3) = \tilde{\chi}_{b_1}(\omega_2, \omega_3) := \tilde{\Phi}(\omega_2, \omega_3) \tilde{e}_{\omega_1}^{\varepsilon_1}(b_1). \quad (6.9b)$$

The observables $\ln(\hat{v}_i)_{b_1}$ are defined as follows. For $i = 2, 3$ we simply act on

$$\chi_{b_1}(v_2, v_3) = \int_{\mathbb{R}^2} d\omega_2 d\omega_3 \tilde{\chi}_{b_1}(\omega_2, \omega_3) e_{\omega_2}^{\varepsilon_2}(v_2) e_{\omega_3}^{\varepsilon_3}(v_3) \quad (6.10)$$

with the kinematical operator $\ln(\hat{v}_i)$. Thus, the action of $\ln(\hat{v}_2)_{b_1}$ on the elements of $\mathcal{H}_{\tilde{e}}^{\text{Phys}}$ turns out to be

$$[\ln(\hat{v}_2)_{b_1} \tilde{\Phi}](\omega_2, \omega_3) = \frac{1}{\tilde{e}_{\omega_1}^{\varepsilon_1}(b_1)} \int d\omega'_2 \langle e_{\omega'_2}^{\varepsilon_2} | \ln(\hat{v}_2) e_{\omega'_2}^{\varepsilon_2} \rangle_{\mathcal{H}_{e_2}^+} \times \tilde{e}_{\omega_1(\omega'_2, \omega_3)}^{\varepsilon_1}(b_1) \tilde{\Phi}(\omega'_2, \omega_3), \quad (6.11)$$

and similarly for $i = 3$. These families are unitarily related by the very same reason explained for $\ln(\hat{v}_a)_{v_1}$ in Sec. VC, and can be extended equally to a complete set of observables.

As an aside, let us comment that in the sLQC approach the analog of the basis eigenfunctions $\tilde{e}_{\omega_1}^{\varepsilon_1}(b_1)$ are pure phases, and then the transformation (6.8) reduces just to a unitary rescaling by $|\omega_2 + \omega_3|^{1/2}$.

The construction of $\ln(\hat{v}_1)_{b_1}$ at a heuristic level is based again on the action of the kinematical operator on some suitable modification of the initial data at b_1 . To give a precise definition, we first need to express the operator $\ln(\hat{v}_1)_{b_1}$ in the b_1 -representation.

Note that the function $\ln(v_1)$ can be expanded around a point $v_1^o > 0$ as

$$\ln(v_1) = \ln(v_1^o) - \sum_{n=1}^{\infty} \frac{1}{n(v_1^o)^n} (v_1^o - v_1)^n. \quad (6.12)$$

Promoting the terms v_1^n to operators and applying relation (6.2), we can represent the operator $\ln(\hat{v}_1)$ as

$$\ln(\hat{v}_1) = \ln(v_1^o) - \sum_{n=1}^{\infty} \frac{1}{n(v_1^o)^n} (v_1^o - 2i\partial_{b_1})^n, \quad (6.13)$$

defined on elements $\chi_{b_1}(v_2, v_3)$ of the kinematical Hilbert space. Changing to the ω_a -representation via Eq. (6.10), the action on $\tilde{\chi}_{b_1}(\omega_2, \omega_3)$ can be expressed as

$$[\ln(\hat{v}_1) \tilde{\chi}_{b_1}](\omega_2, \omega_3) = \tilde{\Phi}(\omega_2, \omega_3) [\ln(\hat{v}_1) \tilde{e}_{\omega_1}^{\varepsilon_1}](b_1), \quad (6.14)$$

and thus the final form of these observables reads:

$$\begin{aligned} \ln(\hat{v}_1)_{b_1}: \mathcal{H}_{\varepsilon}^{\text{Phys}} &\rightarrow \mathcal{H}_{\varepsilon}^{\text{Phys}}, \\ [\ln(\hat{v}_1)_{b_1} \tilde{\Phi}](\omega_2, \omega_3) &= \frac{[\ln(\hat{v}_1) \tilde{e}_{\omega_1}^{\varepsilon_1}](b_1)}{\tilde{e}_{\omega_1}^{\varepsilon_1}(b_1)} \tilde{\Phi}(\omega_2, \omega_3), \end{aligned} \quad (6.15)$$

with $\ln(\hat{v}_1)$ given in Eq. (6.13).

One can check by inspection that these observables are not related by a unitary operator $\hat{Q}_{b_1, b_1^*}: \mathcal{H}_{\varepsilon}^{\text{Phys}} \rightarrow \mathcal{H}_{\varepsilon}^{\text{Phys}}$, analogous to the operators defined in Eq. (5.13). Therefore, the observables $\ln(\hat{v}_1)_{b_1}$ can play only an auxiliary role with respect to the families of unitarily related observables $\ln(\hat{v}_a)_{b_1}$. In the next section we employ these families of observables to analyze the dynamics of physical states which are semiclassical at late times.

C. Numerical analysis

Let us briefly discuss the numerical methods used in our calculations. This is a technical subsection that can be safely skipped if the reader is not interested in the numerics.

As in Sec. V, we concentrate our study on the Gaussian states (4.14). In most cases, the calculations are exactly the same as those of Sec. VD for the observables associated with v_1 -slices. In particular, to compute the expectation values and dispersions of $\ln(\hat{v}_a)$ we have used the analogs of Eqs. (5.15), (5.16), (5.17), (5.18), and (5.19), replacing $\chi_{v_1}^s$ with χ_{b_1} . The eigenfunctions $\tilde{e}_{\omega_1}^{\varepsilon_1}$, needed to determine $\tilde{\chi}_{b_1}$, have been computed via Eq. (6.5) by means of a FFT algorithm. In comparison with Sec. VD, the only relevant difference appears in the calculation of $\langle \ln(\hat{v}_1)_{b_1} \rangle$ and $\langle \Delta \ln(\hat{v}_1)_{b_1} \rangle$, which is performed as follows.

In a first step, we calculate the action of $\ln(\hat{v}_1)_{b_1}$ on $\tilde{\Phi}$ using Eq. (6.15). To find the values of $\ln(\hat{v}_1) \tilde{e}_{\omega_1}^{\varepsilon_1}$, we act with $\ln(\hat{v}_1)$ in the v_1 -representation, and transform the result to the b_1 -representation via Eq. (6.1) by applying a FFT.

At this stage, however, it is necessary to comment on a technical subtlety. In order to calculate the desired result exactly as specified in the previous subsection, one has to normalize the eigenfunction according to Eq. (6.8) before acting on it with $\ln(\hat{v}_1)$. Since the normalization must be done in the b_1 -representation and the action of the operator is known instead in the v_1 -representation, one would have to carry out a sequence of operations, namely, a Fourier transform, a normalization, and an inverse Fourier transform. Unfortunately, the FFT algorithm used for this assumes that both the function that is transformed and the result are supported on points which are uniformly distributed in the circle. Since, in our case, the support of the eigenfunction is an entire subsemilattice, $^{(4)}\mathcal{L}_{\varepsilon_1}^+$, one should restrict it to a set of the form $^{(4)}\mathcal{L}_{\varepsilon_1}^+ \cap [0, v_{\max}]$ (where $v_{\max}$ has some large value), thus removing the tail, which decays (up to logarithmic factors) as v_1^{-1} . The restriction would give rise to numerical errors which would

manifest themselves near $b_1 = 0$ and $b_1 = \pi$. In turn, this would lead to errors in normalization, which would be amplified through the commented sequence of operations (FFT $\rightarrow$ Normalization $\rightarrow$ FFT), making the results in the large volume regime unreliable.

In order to avoid this problem, we implement a slightly different algorithm. Instead of normalizing $\tilde{e}_{\omega_1}^{\varepsilon_1}$, we first act with $\ln(\hat{v}_1)$ on the nonnormalized eigenfunctions, carrying out the normalization afterwards. That is,

$$\tilde{e}_{\omega_1}^{\varepsilon_1}(b_1) \mapsto \tilde{f}_{\omega_1}^{\varepsilon_1}(b_1) := \frac{[\ln(\hat{v}_1) \tilde{e}_{\omega_1}^{\varepsilon_1}](b_1)}{|\tilde{e}_{\omega_1}^{\varepsilon_1}(b_1)|}. \quad (6.16)$$

Such a method introduces an error owing to the difference between the normalized and nonnormalized functions. However, one can argue that the error can be neglected for semiclassical states peaked around large ω_a^* , using that $\tilde{e}_{\omega_1}^{\varepsilon_1}(b_1)$ can be approximated by its sLQC counterpart in that regime:

$$\begin{aligned} \tilde{e}_{\omega_1}^{\varepsilon_1}(b_1) &\sim |\omega_2 + \omega_3|^{1/2} [e^{i\omega_1 x(b_1)} + O(\omega_1^{-2})], \\ x(b) &:= \ln \left[\tan \left(\frac{b}{2} \right) \right]. \end{aligned} \quad (6.17)$$

Once the functions $\tilde{f}_{\omega_1}^{\varepsilon_1}$ are known, we evaluate the profiles

$$\begin{aligned} [\ln(\hat{v}_1) \chi_{b_1}](v_2, v_3) &= \int_{\mathbb{R}^2} d\omega_2 d\omega_3 \tilde{\Phi}(\omega_2, \omega_3) \tilde{f}_{\omega_1}^{\varepsilon_1}(b_1) \\ &\times e^{\varepsilon_2 v_2} e^{\varepsilon_3 v_3}, \end{aligned} \quad (6.18)$$

integrating in practice the right-hand side over the intervals $\omega_a \in [\omega_a^* - 5\sigma_a^*, \omega_a^* + 5\sigma_a^*]$ via the trapezoid method.

The computed profiles are finally used to calculate the expectation values

$$\begin{aligned} \langle \Phi | \ln(\hat{v}_1)_{b_1} | \Phi \rangle &= \| \chi_{b_1} \|^{-2} \sum_{\tilde{\mathcal{L}}^2} \tilde{\chi}_{b_1}(v_2, v_3) \\ &\times [\ln(\hat{v}_1) \chi_{b_1}](v_2, v_3), \end{aligned} \quad (6.19)$$

where owing to technical limitations the summation was restricted to $\tilde{\mathcal{L}}^2 := (\mathcal{L}_{\varepsilon_2}^+ \cap [0, 4\omega_2^*]) \times (\mathcal{L}_{\varepsilon_3}^+ \cap [0, 4\omega_3^*])$.

The dispersions of these observables are found using the standard relations [similar to Eq. (5.19)]. The expectation values $\langle \Phi | \ln(\hat{v}_1)_{b_1}^2 | \Phi \rangle$ are computed with an algorithm that is fully analogous to the one used for $\langle \Phi | \ln(\hat{v}_1)_{b_1} | \Phi \rangle$.

In our numerical simulations, the number of points selected for the FFT of the eigenfunctions is equal to 2^{17} , distributed uniformly in the set $b_1 \in [0, \pi)$. The simulations have been performed for the same range of parameters as in Sec. VD, that is, for ω_a^* ranging from 2.5×10^2 to 10^3 , and for relative dispersions in ω_a between 0.05 and 0.1. The results of these simulations are discussed in the next subsection.

D. Results

A representative example of the numerical analysis of the Gaussian states is presented in Fig. 4. The general conclusions of this analysis can be summarized as follows:

- (i) The states that are sharply peaked at some initial b_1 remain so during the whole evolution.
- (ii) For small b_1 , the expectation values of the three families of observables $\ln(\hat{v}_i)_{b_1}$ follow classical trajectories corresponding to a universe contracting in the three directions. As b_1 increases and the values of v_i decrease becoming of the order of ω_i^* , we observe a deviation from the classical dynamics which results in independent bounces in *all the three directions*. After each bounce (in direction i), the value of v_i starts growing, and its dynamics quickly approaches that of a classical expanding universe.
- (iii) Through the entire evolution, the genuine quantum trajectories *agree to a good precision* (less than 10% of dispersion) with those corresponding to the classical effective dynamics presented in Appendix B.

The results listed above provide an additional (independent) confirmation of the conclusions presented in Sec. VE. However, the current analysis constitutes a significant improvement with respect to that of Sec. V. Namely, while it is still only in an asymptotic sense that the observables used here possess a well-defined physical interpretation, the accuracy of this interpretation remains fairly good during the entire evolution. Unlike the situation found for $\ln(\hat{a})_{v_i}$, where the observables completely lose a meaningful physical interpretation in some epochs of the evolution, the level of confidence depends now just on the peak values ω_a^* . Furthermore, this level improves as one considers more and more macroscopic universes (larger ω_a^*).

VII. CONCLUSIONS AND DISCUSSION

In this work we have investigated the concept of evolution in LQC. Our main goal has been the construction of a well-defined unitary evolution framework with no reference to a matter field as a clock. We have achieved this by building certain families of unitarily related partial observables, parametrized by geometry degrees of freedom. As a test bed for our study, we have chosen the specific example of a vacuum Bianchi I toroidal (T^3) universe.

Within this model, we have proposed two different constructions of observables, built out of the kinematical operators $\ln(\hat{v}_a)$ with $a = 2, 3$, and parametrized, respectively, by: (i) the affine parameter v_1 corresponding to one of the triad coefficients p_1 , which plays the role of a configuration variable, (ii) its conjugate momentum b_1 . In this way, the role of internal time has been assigned to geometry variables, making its definition independent of the matter content.

In order to develop and test our constructions in an analytically solvable setting, as well as to identify the imprint of the loop quantization in the dynamics, we have first implemented them in the quantum version of the system obtained via the standard methods of geometrodynamics, i.e., in the WDW analog of our LQC model. In both of the LQC and WDW theories, the physical Hilbert space of our model is $L^2(\mathbb{R}^2, |\omega_2 + \omega_3| d\omega_2 d\omega_3)$. The difference between them is captured in the form of the observables.

In the WDW theory the basis elements of the kinematical Hilbert space are, essentially, rotating functions, and owing to this property the unitarity in the evolution is easily achieved both for cases (i) and (ii). Furthermore, all the constructed observables have a neat physical inter-

FIG. 4 (color online). Expectation values and dispersions of the observables $\ln(\hat{v}_i)_{b_1}$ on the Gaussian states [with profile (4.14)] presented in the v_2 - v_1 plane and compared with classical (green lines) and effective (blue dotted line) trajectories. The states are peaked at $\omega_2^* = \omega_3^* = 10^3$ with relative dispersions $\Delta\Theta_2/\Theta_2 = \Delta\Theta_3/\Theta_3 = 0.05$. The phases are, respectively, $\beta^2 = \beta^3 = 0$ for (a) and $\beta^2 = \beta^3 = 0.1$ for (b). The expectation values follow the effective trajectory through all the evolution. In particular, the trajectories before and after the bounce coincide in (a).

pretation as the evaluation of $\ln(v_a)$ at a given moment of v_1 or b_1 , respectively.

The constructions described above have been used to investigate the dynamics of states which are semiclassical at late times, with a sharply peaked Gaussian profile. We have shown analytically that any such state follows the classical trajectory right to the classical singularities, which are thus not resolved. Actually, this lack of singularity resolution has been shown to be a general property of the physical states, not only of the Gaussian ones.

In the case of an LQC model, the situation is more complicated. While in case (ii) we have succeeded in applying the construction tested in the WDW model almost straightforwardly, case (i) has posed a considerable challenge. Both a direct application or a straightforward generalization of the scheme introduced for WDW have resulted in operators which either fail to provide a unitarily related family of observables, or do not encode any physically interesting information about the system.

To overcome this problem, we have used our knowledge of the WDW limit of an LQC state, observing that any limit of this kind contains two types of components, which, respectively, move forward and backward in the evolution parameter. This feature has motivated the introduction of a similar splitting in rotating components of the exact LQC wave functions, which has been defined in a precise manner exploiting the properties of the Fourier transform. The scheme for the construction of observables defined in the WDW case has been applied to each of the components separately and has allowed us to attain the required unitarity in the evolution.

In contrast to the WDW case, where the constructed observables admitted a neat physical interpretation, in LQC, owing to the modifications in the construction necessary to ensure unitarity, the physical interpretation of the operators is clear only in approximate sense. In particular, for case (i) the interpretation of the operators as corresponding to the value of $\ln(v_a)$ at a given v_1 is valid only in the large v_1 limit, and accurate only for part of the evolution. For Gaussian states peaked around some ω_a^* , the interpretation ceases to be acceptable when $v_1 \lesssim 0.2|\omega_1(\omega_2^*, \omega_3^*)|$, a feature that we have seen by exchanging the spatial indexes of the kinematical operators and of the internal time v_1 . Nonetheless in case (ii), while the interpretation is still approximate, its accuracy does not change during evolution (i.e., it does not depend on the value of b_1) and is pretty good for the physically interesting states (peaked at large ω_a^*).

Both constructions, (i) and (ii), have been employed to analyze the dynamics of Gaussian states sharply peaked around large ω_a^* . In case (ii), and in order to bring the analysis to a common setting (v_1 - v_a plane) to facilitate the comparison with (i), an additional family of observables—corresponding to $\ln(v_1)$ at given b_1 —has been constructed. However, these observables are not unitarily related; there-

fore they play only an auxiliary role in the discussion. The numerical analysis reveals the following picture (valid both for case (i) and (ii), unless otherwise stated):

- (i) The considered Gaussian states remain sharply peaked (as far as the relative dispersions of the constructed observables are concerned) through all the evolution.
- (ii) For large $v_1/\omega_1(\omega_2^*, \omega_3^*)$, the expectation values of the observables follow classical trajectories, while for other values of this ratio we have observed deviations which ultimately lead to bounces in v_a .
- (iii) Since the physical interpretation of the observables in case (i) is not reliable for small v_1 , because $v_1/\omega_1(\omega_2^*, \omega_3^*)$ becomes small, we have also performed the analysis in terms of the family of observables of case (ii). This analysis has shown as well the bounce in v_1 .
- (iv) The expectation values of the introduced observables (calculated in the domains where their physical interpretation is valid) agree with the trajectories predicted by the classical effective dynamics presented in Appendix B.

As a consequence, in LQC the singularity, already resolved at a kinematical level, is also resolved dynamically. Furthermore, the above observations imply that, similarly to what occurs in the isotropic system, large semiclassical universes expanding in terms of the coefficients p_i are connected to also large and semiclassical contracting ones via a sequence of bounces which are independent for each direction.

Let us point out that the complication of the numerical problems that one has to solve in the analysis of the vacuum Bianchi I model has not allowed us to probe states as semiclassical as the ones studied in the isotropic case (considered, for example, in Ref. [5]), nor check really the long term evolution of the system. Besides, the numerical analysis has been restricted just to Gaussian states. This analysis alone is not sufficient to conclude that all states that are semiclassical before the bounces stay so after them. However, the semianalytical study of the WDW limit that we have performed for case (i) has shown that, whenever the state has finite expectation values and dispersions for the set of operators (4.27) [and finite expectation values for (4.28)], the relative dispersions of $\ln(v_a)_{v_1}$ in both branches of the evolution are asymptotically equal.

In summary, taking the model of the vacuum Bianchi I universe as an example, we have constructed a notion of unitary evolution in a well-defined way and without any reference to a matter field as a clock. We have achieved this goal by building several families of unitarily related observables, which in turn have allowed us to thoroughly analyze the dynamics of the considered model. The results of this analysis confirm at a genuinely quantum level the robustness of the bounce picture, as well as the preservation of the semiclassicality across the bounces.

To conclude, we would like to comment that the approach presented here pioneers the development of a new methodology, which can be employed whenever one has to analyze the evolution in absence of degrees of freedom that are quantized in a standard way. Therefore, it can be applied in a large variety of polymerically quantized systems. In particular, it is applicable to the quantization carried out in Ref. [10] where, for the analogs of the constructions (i) and (ii), we can use the total volume v defined in that reference and its conjugate momentum b , respectively. Nonetheless, the prescription for the so-called improved dynamics chosen for our study here offers us a precise control over the introduced constructions, inasmuch as the mathematical structure of the system has already been carefully studied in the literature and is known in great detail. Furthermore, it allows to test explicitly the reliability of the results provided by the observables. In particular, in the case of the operators parametrized by v_1 , we have been able to recognize a loss of predictability (at least in terms of a conventional physical interpretation of the observables) by interchanging the roles of internal time and dynamical variable between v_1 and v_a ($a = 2$ or 3), a possibility which is not available in the prescription followed in Ref. [10].

ACKNOWLEDGMENTS

This work was supported by the Spanish MICINN Project FIS2008-06078-C03-03 and the Consolider-Ingenio 2010 Program CPAN (CSD2007-00042). The authors are grateful to W. Kamiński, Javier Olmedo, Parampreet Singh, and José M. Velhinho for discussions. M.M.-B. and T.P. acknowledge financial aid by the I3P Program of CSIC and the European Social Fund, in the case of M.M.-B. under the grant I3P-BPD2006. T.P. also acknowledges financial support by the Foundation for Polish Science under the grant Master and thanks the Perimeter Institute and the Institute of Theoretical Physics of Warsaw University for the hospitality in the period of development of this work. M.M.-B. wants to thank A. E. I. for warm hospitality during part of the period when this work was done.

APPENDIX A: DISPERSION IN THE WHEELER-DEWITT LIMIT: ENSEMBLE OF SECTORS AND FURTHER CONSIDERATIONS

In this appendix, we analyze the behavior of the dispersions in the WDW regime taking into account the eight sectors in which the LQC wave functions have a well-defined limit, rather than considering each of these sectors independently. We want to define the ensemble of those sectors in such a way that the properties of the expectation values and dispersions of the LQC observables are reflected by features of their analogs on that ensemble. To achieve this goal, we note the following properties of the operators $\ln(\hat{v}_a)_{v_1}$:

- (a) Since each operator is defined for a definite value of v_1 , which belongs just to one of the subsemilattices, $(4)\mathcal{L}_{\varepsilon_1}$ or $(4)\mathcal{L}_{\varepsilon_1+2}$, we can consider the states supported on them separately. As a consequence, we can safely consider two independent limits corresponding to the splitting of the support in v_1 .
- (b) For given v_1 , the action of the operator $\ln(\hat{v}_a)_{v_1}$ can be represented as the action of the sum of the respective restrictions to each of the four sectors obtained with the splitting into subsemilattices in the directions $a = 2, 3$.

Applying the calculation method explained in Sec. V D to the expectation values and dispersions, one sees immediately that

- (i) the expectation values of $\ln(\hat{v}_a)_{v_1}$ are arithmetic averages of the expectation values of the restrictions, and
- (ii) the dispersions are bounded by an arithmetic average of the dispersions of each of the four contributing sectors plus terms of the form $\sqrt{\langle \hat{D}_m^2 \rangle}$, where the operator $\hat{D}_m$ measures the difference between the total expectation value and that of the considered sector, labeled by $m = 1, \dots, 4$.

On the other hand, in Sec. IV C we proved that, for each of the sectors, the relative dispersion of $\ln(\hat{v}_a)_{v_1}$ ($a = 2, 3$) is the same in the two components moving forward/backward in time, respectively, provided that some mild conditions (e.g.) on the forward-moving component are satisfied. In order to extend the result to the ensemble of sectors, one has to cope with the possible differences between the expectation values of $\ln(\hat{v}_a)_{v_1}$ mentioned above in point (ii).

To verify the boundedness of these differences we observe that the relation between the restrictions of the eigenfunctions to the subsemilattices corresponding to the different sectors under consideration—which is encoded in Eq. (40) of Ref. [9]—, together with the relation between the normalization of these restrictions and that of their WDW limits, imply that the coefficients A_a and W_a are equal for all the studied sectors [see Eqs. (3.19a) and (3.22a)]. From the invariance of these coefficients under the transformation $\tilde{\Phi}_- \rightarrow \tilde{\Phi}_+$ and the considerations made in Sec. IV C, it follows then that the analyzed differences have indeed a well-defined, finite limit as $v_1 \rightarrow \infty$.

We also note that, as in the case of the discussion of Sec. IV C, the above arguments can be repeated considering the transformation $\tilde{\Phi}_+ \rightarrow \tilde{\Phi}_-$, opposite to the one that we have studied here.

Finally, it is worth commenting that the requirement that the state have finite expectation values and dispersions with respect to the operators $\Omega_a^{(2)}$, although providing a restriction on the space of states, can be considered quite reasonable from a physical viewpoint. Actually, since the choice of v_1 as an emergent time (and hence the role of ω_1 as a

“time frequency”) is arbitrary, one can exchange the roles of ω_1 and ω_2 and, for a given state represented by $\tilde{\Phi}(\omega_2, \omega_3)$, consider its transformation into a different one

$$\tilde{\Phi} \rightarrow \tilde{\Phi}': \tilde{\Phi}'(\omega_2, \omega_3) = \tilde{\Phi}(\omega_1(\omega_2, \omega_3), \omega_3). \quad (\text{A1})$$

On the other hand the transformation

$$\tilde{\Phi}(\omega_2, \omega_3) \mapsto \frac{\omega_1^2(\omega_2, \omega_3)}{\omega_2^2} \tilde{\Phi}(\omega_1(\omega_2, \omega_3), \omega_3) \quad (\text{A2})$$

corresponds just with swapping the coordinate v_1 for v_2 . Similar transformations can be defined also for the interchange $v_1 \leftrightarrow v_3$. Combining both of them one can rewrite the square of $\Omega_a^{(2)}$ as the square of $\ln|\omega_2|$ acting on the state represented by $\tilde{\Phi}'$. Therefore, since that square is the main component of the dispersion, one can relate $\langle \Delta \Omega_a^{(2)} \rangle$ with the dispersion of the operator $\ln|\omega_a|$ on $\tilde{\Phi}'$ at least heuristically. Similar arguments can be applied as well to $\Sigma_a^{(2)}$.

APPENDIX B: EFFECTIVE CLASSICAL DYNAMICS

The quantum dynamics resulting from the LQC approach turns out to be surprisingly well reproduced by certain classical effective dynamics, constructed by replacing the holonomies and fluxes in the quantum Hamiltonian constraint by their expectation values [17,18]. This in principle naive construction has been proven to accurately mimic the genuine quantum evolution (with discrepancies much smaller than the quantum dispersions) in several situations (see e.g. [5,14,40]). We sketch here its derivation for the case of the vacuum Bianchi I model.

We start with the quantum constraint (2.5), applying to it the replacements explained above. The resulting effective Hamiltonian takes the form

$$H^{\text{eff}} = -\frac{2}{\gamma^2} [\Theta_1^{\text{eff}} \Theta_2^{\text{eff}} + \Theta_1^{\text{eff}} \Theta_3^{\text{eff}} + \Theta_2^{\text{eff}} \Theta_3^{\text{eff}}], \quad (\text{B1a})$$

$$\Theta_i^{\text{eff}} := 6\pi\gamma G v_i \sin(b_i), \quad (\text{B1b})$$

where the variable b_i ($i = 1, 2, 3$) is the momentum conjugate to v_i [see Eqs. (3.24) and (3.25)]. This momentum is compactified as the unit circle.

Given the Hamiltonian (B1), one can easily derive the Hamilton-Jacobi equations for $\partial_\tau v_i$ and $\partial_\tau b_i$, where τ is a time parameter associated with the Hamiltonian. Defining the constants of motion $\Theta_i^{\text{eff}} = 8\pi\gamma G \mathcal{K}_i$ and $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2 + \mathcal{K}_3$ (as in Ref. [24]) we have

$$(\partial_\tau v_i)^2 = 9(8\pi G)^4 (\mathcal{K} - \mathcal{K}_i)^2 \left[v_i^2 - \left(\frac{4\mathcal{K}_i}{3} \right)^2 \right], \quad (\text{B2a})$$

$$\partial_\tau b_i = 3(8\pi G)^2 (\mathcal{K}_i - \mathcal{K}) \sin(b_i). \quad (\text{B2b})$$

Equation (B2b) immediately implies that, within the intervals $b_i \in [0, \pi)$ and $b_i \in [\pi, 2\pi)$, which in the LQC quantization correspond to the respective subsemilattices $^{(4)}\mathcal{L}_{\varepsilon_i}^+$ and $^{(4)}\mathcal{L}_{\varepsilon_i+2}^+$ (see Sec. VI), each of the variables b_i provides a good candidate for an internal time. On the other hand, the general solution to Eq. (B2a) reads

$$v_i(\tau) = \frac{4}{3} \mathcal{K}_i \cosh[3(8\pi G)^2 (\mathcal{K} - \mathcal{K}_i)(\tau - \tau_o)], \quad (\text{B3})$$

where τ_o is a constant representing the time of the bounce. Therefore, v_i is not monotonous in time.

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