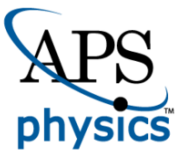

Positive cosmological constant in loop quantum cosmology

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Positive cosmological constant in loop quantum cosmology

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The k=0 Friedmann Lemaitre Robertson Walker model with a positive cosmological constant and a massless scalar field is analyzed in detail. If one uses the scalar field as relational time, new features arise already in the Hamiltonian framework of classical general relativity: In a *finite* interval of relational time, the universe expands out to infinite proper time and zero matter density. In the deparameterized quantum theory, the true Hamiltonian now fails to be essentially self-adjoint both in the Wheeler DeWitt (WDW) approach and in LQC. Irrespective of the choice of the self-adjoint extension, the big bang singularity persists in the WDW theory while it is resolved and replaced by a big bounce in loop quantum cosmology (LQC). Furthermore, the quantum evolution is surprisingly insensitive to the choice of the self-adjoint extension. This may be a special case of an yet to be discovered general property of a certain class of symmetric operators that fail to be essentially self-adjoint.

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I. INTRODUCTION

Loop quantum cosmology (LQC) of the k=0, $\Lambda = 0$ Friedmann Lemaitre Robertson Walker (FLRW) model with a massless scalar field was discussed in detail in [1]. The scalar field serves as a viable internal time variable both in the classical and the quantum theory, with respect to which relational observables such as the matter density and curvature evolve [2, 3]. This makes it possible to explicitly construct the physical Hilbert space and introduce relational Dirac observables to unravel physics of the Planck regime in a large number of cosmological models [4], and a scheme has been sketched even for full general relativity [5]. Using this setup it was rigorously established that, while the big bang singularity persists in the WDW theory of the k=0, $\Lambda = 0$ model, it is resolved due to the quantum geometry effects of loop quantum gravity (LQG) [1].[1]

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[1] Recently, this result has been conceptually sharpened using the consistent histories framework in which one can calculate probabilities for the occurrence of certain histories without recourse to external measurement devices or interaction with environment. Using appropriate coarse grained histories which completely

An appendix in [1] also outlined how the cosmological constant Λ with either sign can be incorporated. A subsequent, detailed discussion of the $\Lambda < 0$ case appeared in [8]. It firmly established that, as in the $\Lambda = 0$ case, in LQC the big bang singularity is replaced by a quantum bounce which occurs when the total energy density $\rho_{\rm tot}$ reaches its maximum value $\rho_{\rm max}$. Furthermore the numerical value of $\rho_{\rm max}$ is the same as in the $\Lambda = 0$ case, $\rho_{\rm max} \approx 0.41\rho_{\rm Pl}$, although now $\rho_{\rm tot}$ includes a contribution from the cosmological constant in addition to the matter density ρ; $\rho_{\rm tot} = \rho + \Lambda/8\pi G$. It turns out that, by a suitable choice of time variable (or lapse function), the $\Lambda = 0$ model can be solved exactly [9]. This is not the case for $\Lambda \neq 0$. Therefore, results of [8] for the $\Lambda < 0$ case are conceptually important also because they demonstrate that the LQC bounce and the qualitative features of the resulting Planck scale physics are not tied to exact solvability. Finally, although the situation with the bounce is the same, the presence of the cosmological constant does alter the underlying mathematical structure in non-trivial ways. In particular, in the deparameterized picture, while the spectrum of the true Hamiltonian is continuous in the $\Lambda = 0$ case, it is purely discrete in the $\Lambda < 0$ case.

The goal of this paper is to present an analogous, detailed account of the $\Lambda > 0$ case. Even though we will again consider a massless scalar field, rather surprisingly, the flip of the sign of the cosmological constant changes the underlying mathematical and conceptual structure significantly. Let us begin with the classical theory. If one again uses the scalar field ϕ for internal time, in contrast to the $\Lambda = 0$ and $\Lambda < 0$ cases [1, 8], the Hamiltonian vector field on the phase space is now incomplete. As a result, volume of any compact co-moving region becomes infinite and the matter density vanishes at a finite instant ϕ_o of internal time ϕ. This situation is qualitatively similar to that in the case of a non-relativistic particle in a steep negative potential whose dynamical trajectories reach infinity in a finite time. In such situations, typically, the Hamiltonian operator in Schrödinger quantum mechanics is symmetric but not essentially self-adjoint. Each self-adjoint extension then yields a unitary evolution but evolutions obtained from distinct operators are both mathematically and physically inequivalent. In the present case, one again finds that the true Hamiltonian operator generating evolution in the scalar field time is symmetric but not essentially self-adjoint. However, rather surprisingly, this ambiguity has negligible effect on states of physical interest: those that start out being peaked at a classical solution in a low curvature region. In particular, all these states undergo a quantum bounce and the total density $\rho_{\rm tot}$ at the bounce is again universal. Furthermore, while the evolution of expectation values of physical observables does depend on the choice of self-adjoint extension, the dependence is extremely weak. This robustness may be related to the fact that, on the classical phase space, one can extend both the evolution equations and the solutions simply by analytical continuation, without having to introduce specific boundary conditions at infinity. Our analysis raises the possibility that there may well be a general pattern and new results could be found on properties of certain sub-classes of operators that fail to be essentially self-adjoint.

The paper is organized as follows. In Sec. II we discuss the Hamiltonian framework for the k=0, $\Lambda > 0$ model. Sec. III is devoted to the WDW quantum theory and Sec. IV to LQC. We conclude in V with a brief summary and discussion. Because the numerical

decohere, it was shown that the probability of encountering a singularity in the distant past or future is 1 in the WDW theory and 0 in LQC for any state (which is in the domain of operators used to construct coarse-grained histories) [4, 6, 7].

simulations in this paper were completed soon after the initial analysis in [1], they use an older value of LQC area gap which turned out to be half the value that is relevant for states used in LQC [10]. In the main text we use this more recent value. Therefore, unfortunately, in Sec. IV there is an occasional mismatch of factors of two between the text and the figures.

II. HAMILTONIAN FRAMEWORK

Because our primary focus is on LQC, in this section we will summarize the phase space formulation of the FLRW model under consideration in terms of variables that descend from LQG. (For details, see, e.g. [4]). The space-time manifolds $\mathcal{M}$ will be taken to be topologically $\mathbb{R}^4$, equipped with a preferred foliation by spatially homogeneous and isotropic space-like slices M. The space-time metrics g will have the form

$$g = -N^2 \mathrm{d}t^2 + a^2(t)\, q^o \tag{2.1}$$

where q^o is the fixed, positive definite, flat metric on M (determined by the co-moving coordinates), N is the lapse function and $a(t)$ the scale factor. Since all physical fields in the model are spatially homogeneous, and since M is non-compact, integrals representing the symplectic structure and Hamiltonians trivially diverge. One therefore introduces an infrared regulator —a cell $\mathcal{C}$ taken to be cubical with sides along co-moving coordinates— and restricts all integrals to it. The phase space structure and intermediate results depend on the choice of $\mathcal{C}$ and q^o. Therefore one has to either show that the *final* physical results are independent of these choices or remove the infrared regulator by letting $\mathcal{C}$ to expand out to fill M.

In LQG, one uses triads in place of 3-metrics. The freedom in the choice of their orientation enables one to introduce a configuration variable v which captures both the volume V of the cell $\mathcal{C}$ determined by q and the orientation of the underlying physical triad:

$$(\mathrm{sgn}\, v)\; v = \frac{V}{2\pi\gamma\lambda\ell_{\mathrm{Pl}}^2} \equiv \frac{a^3 V_o}{2\pi\gamma\lambda\ell_{\mathrm{Pl}}^2} \tag{2.2}$$

where γ is the Barbero-Immirzi parameter of LQG, $\lambda^2 = 4\pi\sqrt{3}\gamma\,\ell_{\mathrm{Pl}}^2$ is the 'area gap' of LQG that is relevant to LQC [10] and V_o the volume of $\mathcal{C}$ with respect to q^o. (sgn v is positive if the physical triad is oriented along the fiducial triad compatible with q^o and negative if the orientations are opposite.) The canonically conjugate momentum is denoted by b. On classical solutions, it is given by

$$b = \gamma\lambda H \;\equiv\; \gamma\lambda \frac{1}{a}\frac{\mathrm{d}a}{\mathrm{d}t} \tag{2.3}$$

where H is the Hubble parameter and t is the proper (or cosmological) time. In these definitions, factors involving γ, λ and ℓ_{Pl} are introduced to simplify the final expression of the Hamiltonian constraint operator later on.[2] For the scalar field, the basic canonical pair

[2] The variable v is the same as that used in [1] and is related to the variable ν of [4, 9] via: $\nu = \lambda v$ and the variable b is related to b used in [4, 9] via $\mathrm{b} = (1/\lambda)b$. These relative rescalings by λ make the variables v, b used here dimensionless which renders a considerable algebraic simplification in various expressions and equations.

is, as usual, $\phi, p_{(\phi)}$. Thus the phase space is topologically $\mathbb{R}^4$ and equipped with basic Poisson brackets:

$$\{b,\, v\} = \frac{2}{\hbar}, \quad \text{and} \quad \{\phi, p_{(\phi)}\} = 1\,. \tag{2.4}$$

Because of a gauge fixing tailored to spatial homogeneity and isotropy, the Gauss and the diffeomorphism constraints of LQG are automatically satisfied [11]. Thus, we are left only with the Hamiltonian constraint. Since we want to use the scalar field ϕ as internal time and since ϕ satisfies the wave equation on $(\mathcal{M}, g)$, it is appropriate to use the lapse field N that is adapted to a harmonic time coordinate τ, satisfying $\Box\tau = 0$ [4]. As in [9], this is achieved by setting $N := a^3$. Then the Hamiltonian constraint is given by:

$$C = \, p^2_{(\phi)} - 3\pi\hbar^2 G b^2 v^2 + \pi\gamma^2\lambda^2\,\hbar^2 G\,\Lambda\, v^2 \;\approx\; 0, \tag{2.5}$$

Note that while $b \in (-\infty, \infty)$, on the constraint surface it must satisfy $|b| \geq b_o = \gamma\lambda\sqrt{\Lambda/3}$. The equations of motion for the scalar field, generated by the Hamiltonian constraint, are:

$$\frac{\mathrm{d}p_{(\phi)}}{\mathrm{d}\tau} = 0 \quad \text{and} \quad \frac{\mathrm{d}\phi}{\mathrm{d}\tau} = 2p_{(\phi)}, \tag{2.6}$$

Eq. (2.6) implies that $p_{(\phi)}$ is a constant in any solution and $\phi(\tau) = 2p_{(\phi)}\tau + \text{const}$. Therefore, in any space-time defined by a phase space dynamical trajectory, ϕ can be used as an evolution parameter in place of τ. This is our relational time variable. The equation of motion for v in the relational time ϕ is given by

$$[\partial_\phi v]^2 = 12\pi G\,[v^2 \,+\, \frac{\pi\gamma^2\lambda^2\ell^2_{\mathrm{Pl}}\hbar\Lambda}{2p^2_{(\phi)}}\, v^4]\,. \tag{2.7}$$

and its solution, expressed in terms of the physical volume $V = (2\pi\gamma\lambda\ell^2_{\mathrm{Pl}})\,|v|$ of the cell $\mathcal{C}$ is:

$$V(\phi) = \big(\frac{\sqrt{4\pi G}\,p_{(\phi)}}{\sqrt{\Lambda}}\big)\;\frac{1}{|\sinh[\sqrt{12\pi G}\,(\phi - \phi_o)]|} \tag{2.8}$$

where ϕ_o is a constant (that can vary from solution to solution). Eq. (2.8) implies that for each ϕ_o we have two types of solutions: Those that start at $\phi = -\infty$ with a big bang singularity, i.e. with zero volume for the cell $\mathcal{C}$, and expand out to infinite volume at $\phi = \phi_o$, and those that start out at infinite volume at $\phi = \phi_o$ and contract into a big crunch singularity at $\phi = \infty$ where $\mathcal{C}$ shrinks to zero volume. In either case, the evolution ends at the finite value ϕ_o of the relational time ϕ. Put differently, the Hamiltonian vector field generating evolution in ϕ is incomplete.

An obvious question then is: Can the phase space evolution be naturally extended beyond $\phi = \phi_o$? We will now show that a mathematically natural extension does exist. Consider first matter density $\rho = p^2_{(\phi)}/2V^2$ of the scalar field, which is a physical observable of direct physical interest. Its time dependence is given by

$$\rho(\phi) = \frac{\Lambda}{8\pi G}\,\sinh^2[\sqrt{12\pi G}(\phi - \phi_o)]\,. \tag{2.9}$$

Since it is analytic in ϕ, in the ρ-ϕ plane the dynamical trajectory represented by the 'contracting branch' is simply an analytical continuation of 'expanding branch'. In space-time terms the full phase space trajectory can be interpreted as follows: the universe starts

out with a big bang at $\phi = -\infty$, expands out till the matter density ρ becomes zero at $\phi = \phi_o$, and then starts contracting, ending in a big crunch at $\phi = \infty$. Situation is similar with respect to b. The dynamical trajectory in the b-ϕ plane also extends analytically from the expanding to the contracting branch:

$$b(\phi) = \pm\, b_o\, \cosh[\sqrt{12\pi G}(\phi - \phi_o)] \quad \text{where} \quad b_o := \gamma\lambda\, \sqrt{\Lambda/3}\,. \tag{2.10}$$

Indeed, in both these cases, it seems artificial to stop the evolution of the expanding branch at $\phi = \phi_o$ and say that the contracting branch, $\phi \geq \phi_o$, is a distinct trajectory.

In the space-time picture, on the other hand, as ϕ approaches ϕ_o, the proper time goes to ∞ in the expanding branch and $-\infty$ in the contracting branch. Therefore the space-time represented by the expanding branch is future complete and that represented by the contracting branch is past complete. In effect, the extended space-time can be obtained by gluing together future null infinity of the expanding branch with the past null infinity of the contacting branch. From the perspective of space-time geometry, this gluing is just an optional mathematical construct. From the perspective of the Hamiltonian framework based on the relational time, on the other hand, the extension is natural and even appears to be necessary to have a complete picture of evolution. Since the Hamiltonian framework can be regarded as the imprint left on the classical regime by the quantum theory, one may suspect that the extension may have its true origin in the mathematical and conceptual framework underlying quantum cosmology. In the next two sections we will see that this is indeed the case.

III. THE WHEELER-DEWITT THEORY

In this section we will first introduce the kinematical structure of the WDW quantum theory, then investigate properties of the operator Θ_Λ representing the gravitational part of the Hamiltonian constraint and finally discuss dynamics. As mentioned in section I, because of the presence of a positive cosmological constant, Θ_Λ fails to be essentially self-adjoint. Much of the discussion is devoted to establishing this property and exploring its consequences.

A. Quantum kinematics

In the Dirac program of quantization of constrained systems, one first ignores the constraints and constructs a kinematical Hilbert space $\mathcal{H}_{\rm kin}$, the quantum analog of the full phase space of the classical theory. The quantum constraint is then written as an operator on $\mathcal{H}_{\rm kin}$. Physical states lie in the kernel of this operator.

In the WDW theory, one takes the kinematic Hilbert space to be $\underline{\mathcal{H}}_{\rm kin} = \underline{\mathcal{H}}_{\rm gr} \otimes \underline{\mathcal{H}}_\phi$, where, as is common in the LQC literature [4], under-bars emphasize that the symbols refer to the WDW theory. As in the textbook Schrödinger quantum mechanics, one sets $\underline{\mathcal{H}}_\phi = L^2(\mathbb{R}, {\rm d}\phi)$ and $\underline{\mathcal{H}}_{\rm gr} := L^2_S(\mathbb{R}, {\rm d}v)$. Here the subscript S denotes that the states are symmetric, i.e., satisfy $\underline{\psi}(v) = \underline{\psi}(-v)$, thereby encoding the fact that since $v \to -v$ results from an orientation flip of the physical triad E^a_i, it is a large gauge transformation [3] under which physics of the model does not change. For later purposes we note that the inner

product between two states $\underline{\psi}, \underline{\chi}$ on the gravitational Hilbert space $\underline{\mathcal{H}}_{\rm gr}$ is given simply by

$$\langle \underline{\psi} | \underline{\chi} \rangle = \int_{\mathbb{R}} \mathrm{d}v \, \underline{\bar{\psi}}(v) \underline{\chi}(v). \tag{3.1}$$

It is straightforward to write down the quantum operator corresponding to the constraint function (2.5):

$$\underline{\hat{C}} \;=\; \mathbb{I} \otimes \partial_\phi^2 + \underline{\Theta}_\Lambda \otimes \mathbb{I} \qquad \text{with} \tag{3.2}$$

$$\underline{\Theta}_\Lambda := \underline{\Theta}_o - \pi G \gamma^2 \lambda^2 \Lambda v^2 \, \mathbb{I} \qquad \text{and} \quad \underline{\Theta}_o = -12\pi G \sqrt{|v|} \partial_v |v| \partial_v \sqrt{|v|}\,, \tag{3.3}$$

where in the expression of $\underline{\Theta}_o$ we have chosen a factor ordering that is compatible with the one used in LQC in section IV (see [1] for details).

Physical states lie in the kernel of $\underline{\hat{C}}$. To find this kernel and endow it with a Hilbert space structure, it is natural to use the general 'group averaging method' [12–14] as in [3, 15]. The implementation requires that the operator $\underline{\Theta}_\Lambda$ be self-adjoint and uses its spectral decomposition. In the $\Lambda \leq 0$ cases these steps could be readily carried out and the physical sector of the theory could be constructed in a rather straightforward manner [1, 8]. With a positive cosmological constant, on the other hand, it turns out that the eigenfunctions $\underline{\psi}(v)$ of $\underline{\Theta}_\Lambda$ (with real eigenvalues) are Bessel functions of imaginary order. Unfortunately, for our purposes, they are difficult to work with (see for example [16], for their properties). Therefore, it turns out to be more convenient to pass to the dual, b-representation and work with the wave-functions $\underline{\psi}(b)$.

Let $\mathcal{D}$ denote the dense domain in $L^2(\mathbb{R}, \mathrm{d}v)$ consisting of smooth functions which, together with all their derivatives, fall off faster than any polynomial at infinity (i.e. let $\mathcal{D}$ be the Schwartz space). The operator $\underline{\Theta}_\Lambda$ is symmetric on $\mathcal{D}$. Given any state $\underline{\psi}(v) \in \mathcal{D}$, the corresponding wave function in the b representation can be obtained by a Fourier transform. We will set

$$[\underline{\mathcal{F}}\psi](b) = \frac{1}{2\sqrt{\pi}} \int_{\mathbb{R}} \mathrm{d}v \, |v|^{-\frac{1}{2}} \, \psi(v) \, e^{\frac{i}{2} vb}, \tag{3.4}$$

so that, using the fact that $\hat{v}\underline{\psi}(b) = -2i\partial_b \underline{\psi}(b)$ in the b representation, the operator $\underline{\Theta}_\Lambda$ assumes a convenient form:

$$\underline{\Theta}_\Lambda = -12\pi G [\, (b\,\partial_b)^2 - b_o^2 \partial_b^2 \,]\,. \tag{3.5}$$

where $b_o = \gamma\lambda\sqrt{\Lambda/3}$. We will first discuss certain properties of $\underline{\Theta}_\Lambda$ and then use them to construct the physical sector of the theory.

B. Properties of Θ_Λ

1. *Weak solutions to the eigenvalue equation*

To discuss dynamics, we have to extend Θ_Λ to a self-adjoint operator. To analyze existence and uniqueness of these extensions, we need weak solutions to the eigenvalue problem $\underline{\Theta}_\Lambda \underline{\psi}_\zeta = \zeta \underline{\psi}_\zeta$, i.e., distributions $\underline{\psi}_\zeta$ such that

$$(\underline{\psi}_\zeta | \underline{\Theta}_\Lambda^\dagger - \bar{\zeta}\mathbb{I}\,|\underline{\chi}\rangle = 0 \qquad\qquad \forall \underline{\chi} \in \mathcal{D}\;, \tag{3.6}$$

where, as usual, the action $(\underline{\psi}_\zeta|\underline{\chi}\rangle$ of the distribution $(\underline{\psi}_\zeta|$ on the test function $|\underline{\chi}\rangle$ is defined using the Hilbert space inner product on $\mathcal{H}_{\rm gr}$.

Now, because of the factor $|v|^{1/2}$ —introduced to simplify the form of the constraint operator— the form of the inner product in the b representation is not transparent. To spell it out, let us first note that the action of Θ_Λ leaves subspaces containing wave functions $\underline{\chi}$ with support on positive and negative v-axis separately invariant. Therefore, we divide the solutions $\underline{\psi}_\zeta$ to (3.6) into parts $\underline{\psi}^\pm_\zeta$

$$\underline{\psi}_\zeta \mapsto \underline{\psi}^\pm_\zeta = \theta(\pm v)\, \underline{\psi}_\zeta \tag{3.7}$$

by considering the inner product of ψ_ζ with test functions which have support only on the positive or negative parts of the v-line. Since by (3.1) the states supported on $\mathbb{R}^+$ are always orthogonal to the ones supported on $\mathbb{R}^-$ the action of $\underline{\psi}_\zeta$ can be written as

$$\begin{aligned} (\underline{\psi}_\zeta|\underline{\chi}\rangle &= (\underline{\psi}^+_\zeta|\underline{\chi}\rangle_+ + (\underline{\psi}^-_\zeta|\underline{\chi}\rangle_-, \qquad \text{where} \\ (\underline{\psi}^\pm_\zeta|\underline{\chi}\rangle_\pm &:= 4\int_{\mathbb{R}} \mathrm{d}b\, \bar{\underline{\psi}}^\pm_\zeta(b)\ [\pm i\partial_b]\underline{\chi}(b) \qquad \forall \underline{\chi} \in \mathcal{D}\,. \end{aligned} \tag{3.8}$$

With this explicit form of the action of $\underline{\psi}_\zeta$ at hand, we can now solve (3.6). For this, it is convenient to introduce a change of variables to simplify the form of $\underline{\Theta}_\Lambda$. Let us set

$$x := \begin{cases} \arctan(b/\sqrt{|b^2-b_o^2|}), & |b|<b_o, \\ \mathrm{sgn}(b)[\pi/2 - \ln(b_o) + \ln(|b|+\sqrt{|b^2-b_o^2|})], & |b|>b_o. \end{cases} \tag{3.9}$$

or, reciprocally

$$b = \begin{cases} b_o\, \sin x, & |x|<\pi/2, \\ b_o \cosh(|x|-\dfrac{\pi}{2})\,\mathrm{sgn}(x), & |x|>\pi/2. \end{cases} \tag{3.10}$$

where, as before, $b_o := \gamma\lambda\sqrt{\Lambda/3}$. (Recall from section II that, in the classical solutions, $|v|\to\infty$ as $b\to\pm b_o$, or equivalently, as $x\to\pm\pi/2$.) Then, except at points $b=\pm b_o$ we have[3]

$$\underline{\Theta}_\Lambda = -12\pi G\ \mathrm{sgn}(|x|-\pi/2)\ \partial_x^2\,. \tag{3.11}$$

Since $\underline{\Theta}_\Lambda$ is just proportional to the simple operator ∂_x^2 except at $x=\pm\pi/2$, and we are interested in distributional eigenfunctions which are symmetric in x, they are necessarily of the form

$$\underline{\psi}_\zeta(x) \;=\; \begin{cases} A_+ e^{i\sqrt{\zeta}x} + A_- e^{-i\sqrt{\zeta}x}, & x>\frac{\pi}{2} \\ B(e^{\sqrt{\zeta}x}+e^{-\sqrt{\zeta}x}), & |x|<\frac{\pi}{2} \\ A_+ e^{-i\sqrt{\zeta}x} + A_- e^{i\sqrt{\zeta}x}, & x<\frac{\pi}{2} \end{cases} \tag{3.12}$$

for constants $A_\pm, B_\pm$ that satisfy suitable 'gluing conditions'.

To determine these conditions we use the fact that the components $\underline{\psi}^\pm_\zeta$ are independent solutions to (3.6) and apply the decomposition (3.12) of them directly to (3.6), using the form

[3] While Θ_Λ preserves the space of smooth functions of b, on functions of x its action is discontinuous at $x=\pm\pi/2$ because, although b is a smooth function of x, $\mathrm{d}b/\mathrm{d}x = 0$ there. Since we are looking for distributional solutions, this discontinuity is harmless.

(3.8) of the inner product. Splitting the domain of integration of (3.8) onto three intervals $\mathcal{I}_i \in \{\,]-\infty, -\pi/2], [-\pi/2, \pi/2], [\pi/2, \infty[\,\}$ and integrating the resulting expression twice by parts we obtain

$$\begin{aligned}(\underline{\psi}^{\pm}_{\zeta}|\underline{\Theta}^{\dagger}_{\Lambda} - \bar{\zeta}\mathbb{I}|\underline{\chi}\rangle_{\pm} &= \mp 4i \sum_{s\in\pm 1,\sigma\in\{+,-\}} \sigma s \lim_{x\to^{\sigma}(s\pi/2)} \underline{\bar{\psi}}^{\pm}_{\zeta}(x)[\underline{\Theta}_{\Lambda}\underline{\chi}](x) \\ &\mp 48i\pi G \sum_{s\in\pm 1,\sigma\in\{+,-\}} \sigma s \lim_{x\to^{\sigma}(s\pi/2)} \mathrm{sgn}(|x|-\pi/2)[\partial_x \underline{\bar{\psi}}^{\pm}_{\zeta}](x)[\partial_x\underline{\chi}](x) \\ &\pm 4i \sum_{i=1}^{3} \int_{\mathcal{I}_i} \mathrm{d}x\, (\partial_x\underline{\chi})\; [\underline{\Theta}_{\Lambda} - \bar{\zeta}]\underline{\bar{\psi}}^{\pm}_{\zeta}\,, \end{aligned} \tag{3.13}$$

where $x \to^{\sigma} (s\pi/2)$ denotes the limit as x approaches $s\pi/2$ from above if $\sigma = +$ and below if $\sigma = -$. Now, the integrand of the third term on the right hand side vanishes identically because $\underline{\psi}^{\pm}_{\zeta}$ are given by (3.12), and the second term on the right side also vanishes because smoothness (in b) of $\underline{\chi}$ implies that $\partial_x\underline{\chi}$ at $x = \pm\pi/2$. Therefore, only nontrivial contributions to the right side of (3.13) come from the first term. Since $\underline{\Theta}_{\Lambda}\underline{\chi}$ does not generically vanish at $x = \pm\pi/2$ we conclude that *weak solutions to the eigenvalue problem are given by (3.12) where the coefficients are chosen so that* $\underline{\psi}_{\zeta} = \underline{\psi}^{+}_{\zeta} + \underline{\psi}^{-}_{\zeta}$ *is continuous in* $x = \pm\pi/2$ (but not necessarily differentiable).

2. Self-adjoint extensions of $\underline{\Theta}_{\Lambda}$

Deficiency Spaces: The operator $\underline{\Theta}_{\Lambda}$ is symmetric on $\underline{\mathcal{H}}_{\rm gr}$ and the operator $\underline{\Theta}_{o}$ is known to be essentially self-adjoint [17]. However, the cosmological constant term acts like a negative unbounded potential. Therefore, from one's experience with Hamiltonians in non-relativistic quantum mechanics, one would not expect the operator $\underline{\Theta}_{\Lambda}$ to be essentially self-adjoint. Indeed, its LQC counterpart was recently shown to admit a family of inequivalent extensions [18]. We will now show that this general expectation is correct by analyzing *deficiency spaces* [19] of $\underline{\Theta}_{\Lambda}$. For notational simplicity, we will first rescale this operator and consider $\underline{\Theta}'_{\Lambda} = (12\pi G)^{-1}\,\underline{\Theta}_{\Lambda}$.

The deficiency spaces $\mathcal{K}^{\pm}$ are spanned by (kinematically) normalizable solutions $\underline{\psi}^{\pm}$ to equation (3.6) with the eigenvalue $\zeta = \pm 8i$ [4]. Their elements are solutions to (3.11) which are symmetric and everywhere continuous. Therefore, from (3.12) it follows that they take the general form

$$\underline{\psi}^{\pm}(x) = A\, e^{2(1\mp i)|x|} \;+\; B\, e^{-2(1\mp i)|x|}, \tag{3.14}$$

for $|x| > \pi/2$, where A, B are some constants. However, we will now show that only the solutions with $A = 0$ are normalizable. Heuristically this is plausible because the first term on the right hand side diverges as $|x| \to \infty$ while the second goes to zero in this limit. But to establish the result we need to consider the Hilbert space norms. Since the inner product

[4] The deficiency spaces as defined in [19] correspond to the eigenvalues $\zeta = \pm i$, however one can equally work with the spaces corresponding to $\zeta = \pm ir$ where r is any positive real number. We chose $r = 8$ just to simplify notation in subsequent calculations

is simple in the v representation, let us solve the equation directly in that representation. Using $\underline{\Theta}_\Lambda$ from (3.2) we can express $\underline{\psi}^\pm$ as a linear combination of Bessel functions

$$\underline{\psi}^\pm(v) = C\,\frac{Y_{\pm 2(1-i)}(-ic|v|)}{\sqrt{|v|}} + D\,\frac{J_{\pm 2(1-i)}(-ic|v|)}{\sqrt{|v|}}\,. \tag{3.15}$$

Since these functions decay at infinity sufficiently fast, to find if they are normalizable it suffices to focus on their behavior for small v. In this limit, the solution approaches

$$\underline{\psi}^\pm(v) \to E_-\,\frac{e^{-2(1\mp i)\ln|v|}}{\sqrt{|v|}} + E_+\,\frac{e^{2(1\mp i)\ln|v|}}{\sqrt{|v|}}\,, \tag{3.16}$$

whence from the form of the inner product (3.1) it follows that only the solution with $E_- = 0$ is normalizable. Since this normalizable solution goes as $|v|^{3/2}$, its Fourier transform (3.4) is well-defined and square integrable in b. Having established this property, we can now return to the eigenfunctions (3.14) in the x representation. Since $\mathrm{d}b/\mathrm{d}x \sim \sinh(x)$, the normalizable solution $\underline{\psi}(x)$ must have the property that $\int \mathrm{d}x \sinh(x)\,|\underline{\psi}|^2 < \infty$. This condition implies that the normalizable solution is given by (3.14) with $A = 0$.

Setting $A = 0$ and using the symmetry properties of elements of $\underline{\mathcal{H}}_{\rm gr}$ and the continuity property of eigenfunctions we conclude that elements of deficiency subspaces $\mathcal{K}^\pm$ have the form

$$\underline{\psi}^\pm(x) = B\begin{cases} \frac{1}{2}[e^{2(1\pm i)x} + e^{-2(1\pm i)x}], & |x| \le \frac{\pi}{2} \\ \cosh(\pi)\; e^{-(2(1\mp i)|x|-\pi)}, & |x| \ge \frac{\pi}{2} \end{cases} \tag{3.17}$$

for some $B \in \mathbb{C}$. From this it follows immediately that $\mathcal{K}^\pm$ are 1-dimensional.

Self-Adjoint Extensions and their Domains: The fact that $\mathcal{K}^\pm$ are non-empty immediately implies that $\underline{\Theta}'_\Lambda$ admits a family of inequivalent self-adjoint extensions [19]. Elements of this family are labeled by the unitary transformations $U : \mathcal{K}^+ \to \mathcal{K}^-$. In our case they are all of the form

$$U_\alpha : \underline{\psi}^+_o \mapsto e^{i\alpha}\underline{\psi}^-_o, \tag{3.18}$$

where $\underline{\psi}^\pm_o$ are some chosen *normalized* elements of $\mathcal{K}^\pm$. Thus, $\underline{\Theta}'_\Lambda$ admits a 1-parameter family of self-adjoint extensions, labeled by $\alpha \in [0, 2\pi)$. Using theorem X.2 of [19], we conclude that the domains $\mathcal{D}_\alpha$ of these extensions are given by

$$\mathcal{D}_\alpha = \{\underline{\psi} + \underline{\psi}^+ + U^\alpha\underline{\psi}^+;\ \underline{\psi} \in \mathcal{D},\, \underline{\psi}^\pm \in \mathcal{K}^\pm\}\,. \tag{3.19}$$

Up to a constant rescaling, the terms $\psi_\alpha := \underline{\psi}^+ + U^\alpha\underline{\psi}^+ \in \mathcal{D}_\alpha$ that depend on and characterize the extension are given by

$$\underline{\psi}_\alpha(x) = \begin{cases} (1/2)\,[e^{2x}\cos(2x - \alpha/2) + e^{-2x}\cos(2x + \alpha/2)] & , \quad |x| \le \pi/2, \\ \cosh(\pi)e^{-(2|x|-\pi)}\cos(2|x| - \alpha/2), & |x| \ge \pi/2\,. \end{cases} \tag{3.20}$$

Although these functions are continuous, generically, they are not differentiable at $x = \pm\pi/2$. On the other hand, each element $\underline{\psi}$ of $\mathcal{D}$ is differentiable in b and satisfies $[\partial_x\underline{\psi}](x = \pm\pi/2) = 0$. Therefore, for fixed value of α the ratio between the left and right hand derivative of any

element of $\mathcal{D}_\alpha$ is a constant, common for all $\mathcal{D}_\alpha$, depending only on α. Furthermore, the function

$$\beta(\alpha) := \arctan\left(\frac{[\partial_x^- \underline{\psi}_\alpha](x=\pi/2)}{[\partial_x^+ \underline{\psi}_\alpha](x=\pi/2)}\right) \in [0,\pi), \tag{3.21}$$

(where $\partial_x^\pm$ denote derivatives from above and below respectively) is monotonic:

$$[\partial_\alpha \beta](\alpha) = \frac{\cosh(\pi)\sinh(\pi)}{\cosh(2\pi)-\sin(\alpha)} \in [0.498,\ 0.502]. \tag{3.22}$$

Therefore the relation

$$[0,2\pi) \ni \alpha \mapsto \beta(\alpha) \in [0,\pi) \tag{3.23}$$

is a bijection. Thus β provides an alternate labeling of the extensions which is much more convenient as it has a direct interpretation in terms of the discontinuity in the derivatives $\partial_x^\pm \underline{\psi}_\alpha$ at $x = \pm\pi/2$. Therefore, labeling the extension by β allows us to easily identify the eigenfunctions of $\underline{\Theta}_\Lambda$ which span particular extended domain.

To summarize, the symmetric operator $\underline{\Theta}_\Lambda$ defined on the domain $\mathcal{D}$ admits a 1-parameter family of self-adjoint extensions $\underline{\Theta}_{\Lambda,\beta}$, parameterized by $\beta \in [0,\pi)$ with domains given by (3.21). The parameter β directly captures the boundary conditions at $x = pi/2$ satisfied by states in the domain $\mathcal{D}_\beta$ of $\underline{\Theta}_{\Lambda,\beta}$ via (3.21).

Eigenfunctions: Given a self-adjoint extension $\underline{\Theta}_{\Lambda,\beta}$ we can construct the corresponding physical Hilbert space $\underline{\mathcal{H}}^{\rm phy}_\beta$ by group averaging and discuss quantum dynamics. Both these tasks require us to find the eigenfunctions of $\underline{\Theta}_{\Lambda,\beta}$. For this, we first note that, since the operator ∂_ϕ^2 in (3.2) is negative definite, only the positive part of $\underline{\Theta}_{\Lambda,\beta}$ is relevant for the construction of $\underline{\mathcal{H}}^{\rm phy}_\beta$. The general, symmetric eigenspaces of $\underline{\Theta}'_\Lambda$ corresponding to the eigenvalue k^2 are 2-dimensional and are spanned by functions $\underline{\psi}_k$ (where $k \in \mathbb{R}$) of the general form

$$\underline{\psi}_k(x) = A \begin{cases} \cosh(kx), & |x| < \pi/2, \\ \cosh(k\pi/2) e^{ik(|x|-\pi/2)}, & |x| > \pi/2 \end{cases} \tag{3.24}$$

where $A \in \mathbb{C}$. The eigenfunctions spanning the particular extended domain $\mathcal{D}_\beta$ need to satisfy the condition analogous to (3.21). They are therefore given by

$$\underline{\psi}_{\beta,k}(x) = B \begin{cases} \frac{\cos(k\pi/2+\sigma_\beta(k))}{\cosh(k\pi/2)}\cosh(kx), & |x| < \pi/2, \\ \cos(k|x|+\sigma_\beta(k)), & |x| > \pi/2, \end{cases} \tag{3.25}$$

where $B \in \mathbb{R}^+$, $k \in \mathbb{R}^+$ and the phase shift $\sigma_\beta(k)$ satisfies the relation

$$\tan(k\pi/2 + \sigma_\beta(k)) = \frac{\tanh(k\pi/2)}{\tan(\beta)}\,. \tag{3.26}$$

To find the normalization factor B we use an analog of the method used in appendix A2 of [20]. Specifically, first note that, for large $|x|$, $\underline{\psi}_{\beta,k}$ approaches an eigenfunction of $\underline{\Theta}'_{\Lambda=0}$ with a controlled rate of convergence

$$\begin{aligned} &\underline{\psi}_{\beta,k}(x) = \underline{\psi}^o_{\beta,k}(x) + O(e^{-2|\tilde{x}|}), \\ &\underline{\psi}^o_{\beta,k}(x) := B\,\cos[\,k(\ln(2) - \ln(b_o) + \frac{\pi}{2} + \tilde{x}) + \sigma_\beta(k)\,]. \end{aligned} \tag{3.27}$$

where $\tilde{x} = \ln|b|$. Similarly, in the v-representation, we have [16]

$$\underline{\psi}_{\beta,k}(v) = \underline{\psi}^o_{\beta,k}(v) + O(v^2). \tag{3.28}$$

which implies [20] that $\underline{\psi}_{\beta,k}$ and $\underline{\psi}^o_{\beta,k}$ satisfy the same (distributional) normalization conditions. Therefore, the known normalization of $\underline{\psi}^o_{\beta,k}$ [9] and the relation between $\underline{\psi}^o_{\beta,k}(x)$ and $\underline{\psi}^o_{\beta,k}(v)$ determined by (3.4), (3.9) fixes B as

$$B = \frac{1}{\sqrt{2\pi k}}. \tag{3.29}$$

To summarize, for every self-adjoint extension $\underline{\Theta}'_{\Lambda,\beta}$ of $\underline{\Theta}'_\Lambda$ the positive part of its spectrum $\mathrm{Sp}_+(\underline{\Theta}'_{\Lambda,\beta})$ equals the entire positive half $\mathbb{R}^+$ of the real line and is absolutely continuous and non-degenerate. The domain $\mathcal{D}_\beta$ of the operator is spanned by eigenfunctions $\underline{e}_{\beta,k}$, with $k \in \mathbb{R}^+$, given by (3.25), where the coefficient B is fixed by (3.29). The resulting eigenfunctions satisfy the normalization condition

$$(\underline{e}_{\beta,k'}|\underline{e}_{\beta,k}) = \delta(k-k'). \tag{3.30}$$

C. The physical sector

Knowing the self-adjoint extensions of $\underline{\Theta}'_\Lambda$ one can trivially construct all the self-adjoint extensions of $\underline{C}$ by substituting $\underline{\Theta}_\Lambda$ in (3.2) with $\underline{\Theta}_{\Lambda,\beta} = 12\pi G\underline{\Theta}'_{\Lambda,\beta}$. Then, knowing the spectral decomposition of $\underline{\Theta}_{\Lambda,\beta}$ one can find the physical Hilbert space corresponding to each extension by the group averaging [12–14] method as in [3]. The resulting (positive frequency) physical states corresponding to each extension are of the form

$$\underline{\Psi}(x,\phi) = \int_{\mathbb{R}^+} \mathrm{d}k\, \underline{\tilde{\Psi}}(k)\, \underline{e}_{\beta,k}(x)\, e^{i\omega(k)\phi}, \tag{3.31}$$

where $\omega(k) = \sqrt{12\pi G}\, k$. As explained in [3, 9] the physical inner product given by the group averaging procedure reduces to simply

$$\langle\underline{\Psi}_1|\underline{\Psi}_2\rangle = \int_{\mathbb{R}^+} \mathrm{d}k\, \underline{\bar{\tilde{\Psi}}}_1(k)\, \underline{\tilde{\Psi}}_2(k) \quad \text{so that} \quad \mathcal{H}^{\mathrm{phy}} = L^2(\mathbb{R}^+, \mathrm{d}k). \tag{3.32}$$

Knowing this form of physical states, we can introduce as usual [4, 9] the notion of the evolution with respect to the internal time ϕ, and interpret the Hamiltonian constraint as the evolution equation. The resulting unitary evolution of the initial data at $\phi = \phi_o$ is given by

$$\underline{\Psi}(x,\phi_o) \mapsto \underline{\Psi}(x,\phi) = e^{i(\phi-\phi_o)\sqrt{|\underline{\Theta}_{\Lambda,\beta}|}}\ \underline{\Psi}(x,\phi_o)\,, \tag{3.33}$$

where $|\underline{\Theta}_{\Lambda,\beta}|$ is the positive part of $\underline{\Theta}_{\Lambda,\beta}$.

To extract physics from this setup, one needs a family of relational observables on $\underline{\mathcal{H}}_{\mathrm{phy}}$, parameterized by the internal time ϕ. In the cases $\Lambda \leq 0$ [1, 8] this role was served by operators $|\hat{v}|_\phi$ corresponding to the volume (of the fiducial cell $\mathcal{C}$) at given value of ϕ. In our case, however, in the classical theory v becomes infinite at a finite value of ϕ. On the quantum level this property is reflected by the fact that an operator $|\hat{v}|_\phi$ can map even the

elements of the Schwartz space $\mathcal{S} \in \mathcal{H}^{\rm phy}$ outside of $\mathcal{H}^{\rm phy}$. Since the physical origin of this technical problem is clear from the classical analysis, so is the solution: One can simply replace $|\hat{v}|_\phi$ with $|f(\hat{v})|_\phi$, where f is a *bounded* function of v. A convenient choice of f is an 'angular parameter' $\theta \in]0, \pi/2[$ defined by

$$V = K\, \tan(\theta), \tag{3.34}$$

where K is a constant with dimension of the volume. Following the general procedure introduced in [1, 3], one first introduces a kinematical operator acting on the initial data space $P^+_\beta \underline{\mathcal{H}}_{\rm gr}$ consisting of states in $\underline{\mathcal{H}}_{\rm gr}$ in the positive part of the spectrum of $\underline{\Theta}_{\Lambda,\beta}$

$$\big(\hat{\theta}\underline{\psi}\big)(v) = \big(P^+_\beta\ \arctan(\frac{|v|}{K})\, P^+_\beta\, \underline{\psi}\big)(v) \tag{3.35}$$

(P^+_β projects elements $\underline{\psi}(v)$ of $\mathcal{H}_{\rm gr}$ into their positive frequency part by restricting the corresponding Fourier transform $\underline{\tilde{\psi}}(k)$ to the positive half k-line.) In the second step, one extends it to the physical operator $\hat{\theta}|_\phi$ using (3.33):

$$\big(\hat{\theta}|_{\phi_o}\, \Psi\big)(x,\phi) = e^{i(\phi-\phi_o)\,\sqrt{|\underline{\Theta}_{\Lambda,\beta}|}}\ \big(\hat{\theta}\underline{\Psi}\big)(x,\phi_o)\,, \tag{3.36}$$

This relational Dirac observable enables us to effectively track the evolution of volume of the fiducial cell $\mathcal{C}$.

There are other observables which are manifestly independent of the choice of a fiducial cell. An example is provided by the family $|\hat{b}|_\phi$ built out of the kinematical observable $|\hat{b}|$. This observable is of direct physical interest because classically b is proportional to the Hubble rate H: $b = \gamma\lambda\, H$. Finally, another cell-independent observable of direct physical interest is the total energy density $\hat{\rho}_{\rm tot}|_\phi$ commonly used in LQC [9, 15]. It is constructed starting from the kinematical operator

$$\hat{\rho}_{\rm tot} = \frac{1}{2\lambda^2\,(2\pi\gamma G)^2}|\hat{v}|^{-1}\underline{\Theta}_o|\hat{v}|^{-1} = \frac{3}{8\pi G\,\lambda^2\gamma^2}\,\hat{b}^2. \tag{3.37}$$

We will now use this setup to explore quantum dynamics of the WDW theory.

D. Quantum dynamics

Thanks to the simple form of the evolution operator (3.11) and its eigenfunctions (3.25), we can draw some general conclusions regarding quantum dynamics at a semi-heuristic level. Note first that, for $|x| > \pi/2$, every self-adjoint extension $\Theta_{\Lambda,\beta}$ yields a standard Klein-Gordon equation in the x, ϕ plane, with boundary conditions at the 'barrier' $|x| = \pi/2$ defined by that particular choice of β. Most of the wave is reflected at this barrier as the tunneling amplitude is exponentially suppressed. Therefore one would expect the qualitative features of the evolution to be as in Fig.1. Consider a quantum state $\underline{\tilde{\Psi}}(k)$ which is sharply peaked about a large $k^\star$ for which $\underline{\Psi}(x,\phi)$ is peaked on a classical trajectory

$$b(\phi) = b_o\, \cosh[\sqrt{12\pi G}(\phi-\phi_o)] \quad \text{or} \quad x(\phi) = \frac{\pi}{2} + \sqrt{12\pi G}\,(\phi_o - \phi) \tag{3.38}$$

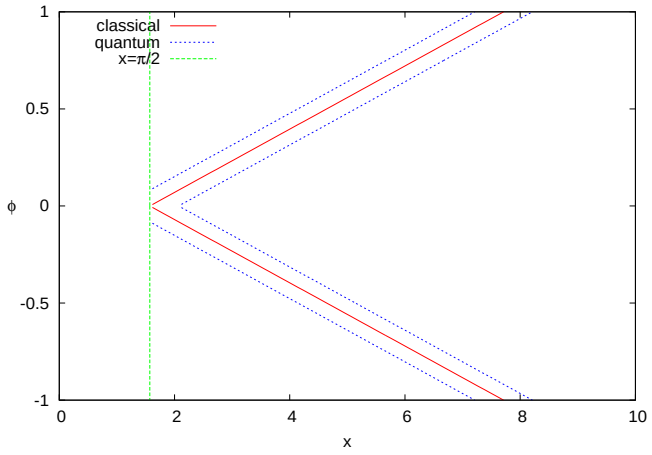

FIG. 1: Qualitative behavior of the quantum evolution can be inferred from the classical dynamics coupled with the form of eigenfunctions. Expanding classical trajectories start at ($x = \infty$, $\phi = -\infty$) (the big bang) and end at ($x = \pi/2$, $\phi = \phi_o$) (where the matter density ρ goes to zero), while the contracting trajectories start at ($x = \pi/2$, $\phi = \phi_o$) and at ($x = \infty$, $\phi = \infty$) (the big crunch). For definiteness we have set $\phi_o = 0$ in the figure. The form of $\underline{\Theta}_{\Lambda,\beta}$ and its eigenfunctions in the x-representation suggest that incoming semi-classical wave functions would be largely reflected at $x = \pi/2$ and follow the contracting classical trajectory which is the analytical continuation of the original one. The figure shows only the part $x > 0$ because the physical states $\underline{\Psi}(x, \phi)$ are symmetric under reflection in x.

in the low curvature region at some $\phi < \phi_o$. Then, because of the reflection at $|x| = \pm\pi/2$, one would expect $\underline{\Psi}(x, \phi)$ to remain sharply peaked on the trajectory

$$x(\phi) = \frac{\pi}{2} + \sqrt{12\pi G}\,|\phi - \phi_o|\,. \tag{3.39}$$

for all ϕ, even to the future of $\phi = \phi_o$. But this is only a qualitative argument because it neglects the tunneling into the region $|x| < \pi/2$ and ignores the k dependence of the reflection coefficients.

To make precise statements regarding the global evolution one has to analyze the expectation values and dispersions of appropriate observables. Since the model is not analytically soluble, one has to resort to numerical methods using a suitable class of states. Following the existing literature, we select the Gaussians sharply peaked about some large $k^\star$ and some $b^\star$ at given initial time $\phi_o \ll -1/\sqrt{G}$. The spectral profiles corresponding to such states are of the type

$$\tilde{\underline{\Psi}}(k) = e^{-\frac{(k-k^\star)^2}{2\sigma^2}}\, e^{-i\omega(k)\phi^\star}, \quad \text{where} \quad \phi^\star := \phi_o + \frac{1}{\sqrt{12\pi G}}\,\mathrm{arcosh}(b^\star/b_o)\,. \tag{3.40}$$

Since the explicit form of the basis functions $\underline{e}_{\beta,k}$ is known via (3.25) and (3.29) the wave function $\underline{\Psi}(b, \phi)$ can be calculated by first carrying out a direct integration of (3.31) and then passing to the b representation using (3.9)).

Recall that the expression of the inner product is quite complicated in the b-representation but extremely simple in the v-representation. On the other hand, the expression of some of the basic operators is simpler in the b-representation. Therefore the calculation requires us

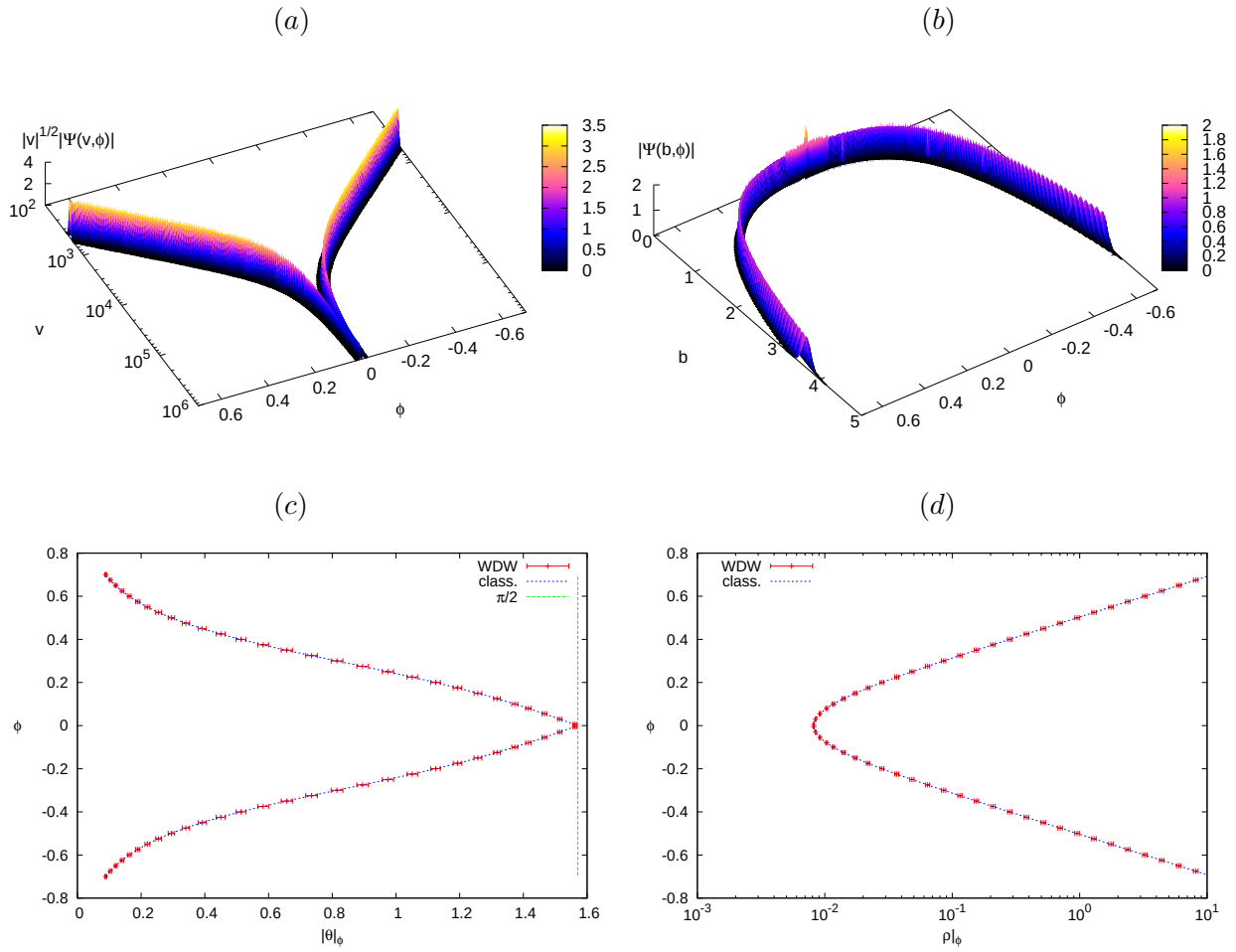

FIG. 2: Quantum dynamics in the WDW theory. Evolution of the wave packet initially peaked at $p_\phi^\star = 5 \times 10^3$ and $|\theta|^\star_{\phi=0} = \pi/2$ with dispersion $\Delta p_\phi/p_\phi = 0.03$. Figures (a) and (b) show the evolution in the v-ϕ and b-ϕ plane, respectively. Figures (c) and (d) show the expectation values of the observables $|\hat{\theta}|_\phi$, and $\hat{\rho}_{\rm tot}|_\phi$ in this state and compare them with the analytically extended classical trajectories. In these simulations, $\beta = 0$, the constant K in the definition of θ was set to $K = 5 \times 10^3$, and $\Lambda = 0.2\ell_{\rm Pl}^{-2}$

to pass between the two representations using the Fourier transform (3.4) and its inverse. Consequently, numerical analysis of dynamics —calculation of the expectation values and dispersions of $\hat{\theta}|_\phi, \hat{\rho}_{\rm tot}|_\phi$— was carried out in the following steps

(i) First, the profiles $\underline{\Psi}(x, \phi)$ at a given ϕ were found via the integration of (3.31) over the interval $k \in [k^\star - 7\sigma, k^\star + 7\sigma]$ via Romberg method with the stepsize and order selected dynamically to achieve the relative integration precision of the order 10^{-6}. The corresponding wave function $\underline{\Psi}(b, \phi)$ was then calculated using (3.10).

(ii) Next, $\underline{\Psi}(b, \phi)$ was used to compute the function

$$\underline{\Phi}(b, \phi) := b^2 \underline{\Psi}(b, \phi). \tag{3.41}$$

that is needed to evaluate the expectation values in step (iv) below.

(iii) Results were transformed to the v-representation via an inverse of (3.4). The Fourier transform involved in it was computed via a Fast Fourier Transform (FFT) algorithm with 2^N probing points (where N varied from 16 to 19). To adapt the resolution in b (corresponding to the size of the domain of calculation in v) the domain of transformation $b \in [-b_M, b_M]$ was allowed to change in the process of evolution and varied from 0.5 to 5.

(iv) Finally the norm, and the expectation values were calculated as follows

$$\|\Psi\|^2 = \int_{\mathbb{R}} \mathrm{d}v |\Psi(v,\phi)|^2, \tag{3.42a}$$

$$\langle |\hat{\theta}|_\phi \rangle = \|\Psi\|^{-2} \int_{\mathbb{R}} \mathrm{d}v \, \arctan(\frac{|v|}{K}) |\Psi(v,\phi)|^2, \tag{3.42b}$$

$$\langle \hat{\rho}_{\rm tot}|_\phi \rangle = C_\rho \|\Psi\|^{-2} \int_{\mathbb{R}} \mathrm{d}v \, \bar{\Psi}(v,\phi)\Phi(v,\phi), \tag{3.42c}$$

where $C_\rho = 3/(8\pi G\,\lambda^2\gamma^2)$. The dispersions were found via a standard relation

$$\delta_O^2 = \langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2 \tag{3.43}$$

for a given observable $\hat{O}$. On the other hand, the expectation values of squared operators are determined via

$$\langle |\hat{\theta}|_\phi^2 \rangle = \|\Psi\|^{-2} \int_{\mathbb{R}} \mathrm{d}v \, \arctan^2(\frac{|v|}{K}) |\Psi(v,\phi)|^2, \tag{3.44a}$$

$$\langle \hat{\rho}_\phi^2 \rangle = C_\rho^2 \|\Psi\|^{-2} \int_{\mathbb{R}} \mathrm{d}v |\Phi(v,\phi)|^2. \tag{3.44b}$$

All the integrations in this step were performed via the trapezoid method, with the configuration of the probing points preset by the FFT in the previous step.

A large number of simulations were performed varying the parameters of the initial state and the self-adjoint extension used in evolution. They bore out the semi-heuristic expectation described in the beginning of this sub-section. An example of the results is presented in Fig. 2. For any choice of extension, states that are sharply peaked in the distant past (or, future) remain so throughout the evolution and follow the analytically extended classical trajectories towards big bang and big crunch singularities. *Thus, as in the $\Lambda = 0$ case, the big bang and the big crunch singularities are not resolved in the* WDW *theory.* The new element is that the wave packets follow the *analytically extended* classical trajectory beyond $\phi = \phi_o$, *irrespective of the choice of the self-adjoint extension.*[5]

Now, usually in quantum mechanics the existence of inequivalent self-adjoint extensions implies that at some point the physical evolution breaks down and additional data are required to continue it. In our case these data correspond to the gluing conditions at $|b| = b_o$ or $|x| = \pi/2$. However, surprisingly, for states which start out as semi-classical in

[5] A previous result in the WDW theory, but using a 'spinor formalism' [21], hinted at the existence of such an extension. Although the scale factor played the role of time there, the quantum wave packet developed a second branch which, in retrospect, may be interpreted as the analog of this extension.

the weak curvature regime, this non-uniqueness does not manifest itself at least at the level of the expectation values of the observables: All of them follow the (analytically extended) classical trajectories dictated by parameters $k^\star, b^\star, \phi^\star$ used in their construction. This result is a reflection at the quantum level of the fact that the classical solutions admit a *unique* analytic extension.

But what about generic wave functions? To better understand the dependence of physical quantities on the choice of extension in this case, let us first consider wave functions in the x variable. For $|x| \geq \pi/2$ each basis function $\underline{e}_{\beta,k}$ has the form of a standing wave and can be decomposed onto the incoming $\underline{e}^-_{\beta k}$ and outgoing $\underline{e}^+_{\beta,k}$ component

$$\underline{e}^\pm_{\beta k} = (1/\sqrt{8\pi k})\, e^{\pm i(k|x|+\sigma_\beta(k))}. \tag{3.45}$$

By replacing $\underline{e}_{\beta,k}$ in (3.31) with $\underline{e}^\pm_{\beta,k}$, we arrive at a split of the wave function $\underline{\Psi}(x,\phi)$ onto expanding $\underline{\Psi}^-$ and contracting $\underline{\Psi}^+$ components. Let us define

$$\underline{e}'^\pm_k(x) = e^{\mp i\sigma_\beta(k)}\ \underline{e}^\pm_{\beta,k}(x) \tag{3.46}$$

by rotating each basis function so that the result $\underline{e}'^\pm_k(x)$ is β-independent and rewrite the expanding and contracting wave functions in terms of them:

$$\underline{\Psi}'^\pm(x,\phi) = \int_{\mathbb{R}^+} \mathrm{d}k\, \underline{\tilde{\Psi}}'^\pm(k)\ \underline{e}'^\pm_k(x)\, e^{i\omega(k)(\phi-\phi_o)}\,. \tag{3.47}$$

Then the spectral profiles $\underline{\tilde{\Psi}}'^\pm$ satisfy

$$\underline{\tilde{\Psi}}'^\pm(k) = e^{\pm i\sigma_\beta(k)}\underline{\tilde{\Psi}}(k)\,, \quad \text{whence} \quad \underline{\tilde{\Psi}}'^+(k) = e^{2i\sigma_\beta(k)}\underline{\tilde{\Psi}}'^-(k)\,. \tag{3.48}$$

Thus upon reflection, the initial expanding wave profile $\underline{\Psi}'^-(k)$ undergoes a phase shift $e^{2i\sigma_\beta(k)}$ that depends on the choice of the self-adjoint extension. Note that the expression (3.26) of σ_β implies that the difference $\sigma_\beta - \sigma_{\beta'}$ in rotations of the phase caused by two different extensions is not global, but depends on k. This subtlety should be reflected in the evolution of observables.

To extract this information, it is convenient to follow [20] and regard the global evolution as a scattering process. For, in the distant past, i.e., $\phi \ll -1/\sqrt{G}$, and in the distant future, i.e. $\phi \gg 1/\sqrt{G}$, we are near the big bang and big crunch singularities where the effect of the cosmological constant can be neglected relative to that of matter, i.e., $\Lambda/8\pi G \ll \rho$. Therefore, in these 'asymptotic' regions, dynamics is better and better approximated by that in the $\Lambda = 0$ case. Thus we can regard 'incoming' and 'outgoing states' as belonging to the $\Lambda = 0$ physical Hilbert spaces. The incoming state can be thought of as being scattered because of the presence of the cosmological constant which dominates dynamics near $|x| = \pi/2$. As in [20], the scattering process can be analyzed using observables $\ln|v|_\phi$. However, it is more convenient to consider observables $\ln|\hat{b}|_\phi$ defined in analogy to $|\hat{b}|_\phi$. The limit of the basis functions is provided already by (3.27). Following our analysis in the x variable, we split this limit into incoming and outgoing components expressed in terms of the basis of $\underline{\Theta}_o$ in the b-representation

$$\underline{e}_{\beta,k}(b) = \frac{1}{\sqrt{2}}\ e^{i(k\beta_o+\sigma_\beta(k))}\ \underline{e}^+_k(b)\ + e^{-i(k\beta_o+\sigma_\beta(k))}\ \underline{e}^-_{-k}(b)\ +\ O(b^{-2})\,, \tag{3.49a}$$

$$\text{with} \quad \underline{e}_k(b) = (1/\sqrt{4\pi|k|})e^{ik\ln|b|}, \tag{3.49b}$$

where $\beta_o := \pi/2 + \ln(2/b_o)$. Using this split in (3.31) we can define the asymptotic future and past states $\underline{\Psi}^{\pm}$ of the spectral profiles:

$$\underline{\tilde{\Psi}}^{\pm}(k) = \theta(\mp k)\, e^{\pm i(|k|\beta_o + \sigma_\beta(|k|))}\, \underline{\tilde{\Psi}}(|k|)\,. \tag{3.50}$$

Now the global evolution is described by the scattering operator $\hat{S}$

$$|\underline{\Psi}^{-}\rangle \;\; \mapsto \;\; |\underline{\Psi}^{+}\rangle = \hat{S}|\underline{\Psi}^{-}\rangle \tag{3.51}$$

where the matrix elements of the scattering operator $\hat{S}$ are given by

$$S(k,k') := (\underline{e}_k|\, \hat{S}\, |\underline{e}_{k'}) \;=\; e^{-2i\,\mathrm{sgn}(k')(\beta_o + \sigma_\beta(|k|))}\; \delta(k+k'). \tag{3.52}$$

The extension dependence is encoded entirely in the phases shift $\sigma_\beta(k)$ given by (3.26). For large k, it can be expanded as

$$\sigma_\beta(k) = -\frac{k\pi}{2} + \frac{\pi}{2} - \beta - \frac{1}{2}\sin(2\beta)e^{-k\pi} + O(e^{-2k\pi})\,. \tag{3.53}$$

Let us now select two extensions corresponding to some β and β' and two states $|\underline{\Psi}\rangle, |\underline{\Psi}'\rangle$ corresponding to those extensions, sharply peaked at some $k^\star$ and such that in the asymptotic past they are equal. Then by (3.51) in the asymptotic future they are related just by a phase rotation

$$\underline{\tilde{\Psi}}^{+}(k) = e^{-2i(\sigma_\beta(k) - \sigma_{\beta'}(k))}\; \underline{\tilde{\Psi}}^{\prime +}(k). \tag{3.54}$$

This allows us to estimate via (3.53) the leading order correction to the difference between the expectation values of $\ln|\hat{b}|_\phi$ as

$$|\langle\underline{\Psi}^{+}|\, \ln|\hat{b}|_\phi\, |\underline{\Psi}^{+}\rangle - \langle\underline{\Psi}^{\prime +}|\, \ln|\hat{b}|_\phi\, |\underline{\Psi}^{\prime +}\rangle| = \pi\cos(\beta+\beta')\sin(\beta-\beta')\, e^{-\pi k^\star} + O(e^{-2\pi k^\star})\,. \tag{3.55}$$

(Since $\underline{\Psi}^{+}$ and $\underline{\Psi}^{\prime +}$ are asymptotic states, i.e. states in the $\Lambda = 0$ theory, the difference is ϕ-independent.) To appreciate the physical implication of this result, let us focus for a moment on semi-classical states peaked at a large $k^\star$ such that initially the dispersions in $\ln|b|$ and $\ln|k|$ are comparable and the uncertainty product is approximately saturated. Then, in either the β or β' theory, because of the Heisenberg uncertainty principle, the dispersion in $\ln|\hat{b}|$ is of the order of $|k^\star|^{-(1/2)}$. Because of the exponential suppression in (3.55), the difference in the expectation values of $\ln|\hat{b}|$ in the β and β' theories is therefore completely negligible compared to the dispersion in $\ln|\hat{b}|$ in either of these theories.

Let us now return to general states. The dependence of dispersions of the choice of self-adjoint extension is slightly stronger than that in (3.55). Results of [20] show that the possible growth of dispersion between the asymptotic past and future states depends on the behavior of $\partial_k\sigma_\beta(k)$. By repeating for the WDW theory the derivation of certain triangle inequalities on dispersions obtained in [20] for LQC, one can shows that the expected difference between the dispersions δ_+ and δ'_+ of $\ln|b|$ for the two states $|\underline{\Psi}^{+}\rangle$, $|\underline{\Psi}^{\prime +}\rangle$ (of the WDW theory now under consideration) will be of the order of

$$\begin{aligned} |\delta_+ - \delta'_+| \;&\lessapprox\; \langle\underline{\Psi}^{+}|\, \Delta(\partial_k(\sigma_\beta - \sigma_{\beta'}))\, |\underline{\Psi}^{+}\rangle \\ &\lessapprox\; |\,[\partial_k^2(\sigma_\beta - \sigma_{\beta'})]\,(k^\star)|\, \sigma_{\ln|k|} \\ &\lessapprox\; \pi^2\,|\,\cos(\beta+\beta')\sin(\beta-\beta')\,|\; e^{-\pi k^\star}\, \delta_{\ln|k|}. \end{aligned} \tag{3.56}$$

where $\delta_{\ln|k|}$ is the dispersion of the observable $\ln|\hat{k}|$. (Here and in what follows the approximate sign in the inequality emphasizes the fact that we are keeping track only the leading order terms.)

Now, the change in the dispersion between the asymptotic past and future state is given by

$$\begin{aligned} |\delta_+ - \delta_-| &\lessapprox 2\langle \underline{\Psi}^+|\, \Delta(\partial_k \sigma_\beta)\, |\underline{\Psi}^+\rangle \\ &\lessapprox 2|\, [\partial_k^2 \sigma_\beta](k^\star)\, |\, \delta_{\ln|k|} \\ &\lessapprox \pi^2 \sin(2\beta)\, e^{-\pi k^\star}\, \delta_{\ln|k|}, \end{aligned} \tag{3.57}$$

where δ_- is the dispersion of the observables $\ln|\hat{b}|_\phi$ on the state $|\underline{\Psi}^-\rangle$. (Again since the asymptotic states refer to the $\Lambda = 0$ theory, this difference is ϕ independent.) Thus, the difference in the dispersions $|\delta_+ - \delta'_+|$ in the asymptotic future in the β and β' theory is comparable to the change in the dispersion $|\delta_+ - \delta_-|$ between asymptotic past and future in any one theory. Both these quantities are *very* small compared to the dispersion $\delta_{\ln|k|}$ in the scalar field momentum.

To summarize, computer simulations of states which start out as Gaussian in the weak curvature region established that the big bang and the big crunch singularities fail to be resolved in the WDW theory. They also brought out the surprising fact that although the final physical sector of the quantum theory does depend on the choice of the self-adjoint extension $\underline{\Theta}_{\Lambda,\beta}$ of the symmetric operator $\underline{\Theta}_\Lambda$, the difference in the dynamics of these states is negligible. The S-matrix strategy first introduced in [20] enabled us to obtain certain analytical inequalities for generic states for which the dispersion in k —i.e., in the field momentum— is finite. They showed that if the dispersion $\delta_{\ln|k|}$ is small, then differences in the S-matrix predictions of physical theories that result from different choices of self-adjoint extensions are enormously suppressed.

IV. LOOP QUANTUM COSMOLOGY

In this section we will show that the procedure followed in Sec. III for the WDW theory can be repeated in a rather straightforward manner for LQC. Therefore our discussion will be parallel to that of Sec. III A and III D with emphasis on the differences from the WDW theory.

A. LQC kinematics

As in the WDW theory, the kinematical Hilbert space is a tensor product $\mathcal{H}^{\rm kin} = \mathcal{H}_{\rm gr} \otimes \mathcal{H}_\phi$. However, while we again have $\mathcal{H}_\phi = L^2(\mathbb{R}, {\rm d}\phi)$, the gravitational Hilbert space is now different [4, 11]. As in the $\Lambda = 0$ case [1], it is given by $\mathcal{H}_{\rm gr} = L^2(\bar{\mathbb{R}}, {\rm d}\mu_{\rm Bohr})$, where $\bar{\mathbb{R}}$ is a Bohr compactification of the real line and ${\rm d}\mu_{\rm Bohr}$ the Haar measure thereon. A convenient basis is again provided by the eigenvectors of the operator $\hat{v}$:

$$\hat{v}|v\rangle = v|v\rangle, \quad \text{so that} \quad \hat{V}|v\rangle = (2\pi\gamma\lambda\ell_{\rm Pl}^2)\, |v|\, |v\rangle\,, \tag{4.1}$$

where, as before, γ is the Barbero-Immirzi parameter of LQG and λ^2 is the LQC *area gap* [10]. As in the WDW theory, in the volume representation states in $\mathcal{H}_{\rm gr}$ become wave

functions $\psi(v)$, which are again taken to be symmetric $\psi(v) = \psi(-v)$ to incorporate the fact that $v \to -v$ is a large gauge transformation corresponding to the flip of the orientation of the physical triad. However, unlike in the WDW theory, the $\psi(v)$ now have support only on a countable set of points along the v-axis and their inner product is given by a sum

$$\langle\psi|\psi'\rangle = \sum_{v\in\mathbb{R}} \bar{\psi}(v)\psi'(v)\,, \tag{4.2}$$

rather than an integral.

Because the Hilbert space is so different, the differential operator $\underline{\Theta}_o = -12\pi G\,\sqrt{|v|}\,\partial_v\,|v|\,\partial_v\sqrt{|v|}$ of the WDW theory fails to be well-defined on $\mathcal{H}_{\rm gr}$. Therefore, one has to first express the classical constraint in terms of the elementary variables of LQG —holonomies and fluxes— and then promote the result to an operator on $\mathcal{H}_{\rm gr}$. This systematic procedure leads to the following form of the constraint operator [1]

$$\hat{C} = \mathbb{I}\otimes\partial_\phi^2 + \Theta_\Lambda\otimes\mathbb{I}, \qquad \Theta_\Lambda := \Theta_o - \pi G\gamma^2\lambda^2\,\Lambda\,v^2\,, \tag{4.3}$$

where

$$-[\Theta_o\psi](v) = f_+(v)\,\psi(v-4) - f_o(v)\,\psi(v) + f_-(v)\psi(v+4)\,, \tag{4.4}$$

with the coefficients $f_{o,\pm}$ given by

$$f_\pm(v) = (3\pi G/4)\,\sqrt{v(v\pm4)}\,(v\pm2), \qquad f_o(v) = (3\pi G/2)v^2\,. \tag{4.5}$$

Thus, the second order differential operator $\underline{\Theta}_o$ of the WDW theory is now replaced by a second order difference operator Θ_o with uniform steps of size $v = \pm4$. Therefore, there is super-selection: one can investigate dynamics separately on uniform lattices in the v-space and each sector consisting of wave functions with support on any one of these lattices is preserved by the complete set of Dirac observables of interest, discussed in section III. In this paper, we will restrict ourselves to the lattice $\mathcal{L} = \{v = 4n,\, n \in \mathbb{Z}\}$ for simplicity because in LQC physical results are largely insensitive to the choice of the sector [22].

Finally, as in the WDW theory, for technical reasons it is more convenient to work in the dual representation in which states are wave functions $\psi(b)$ of the conjugate variable b. However, since the LQC states $\psi(v)$ have support only at $v = 4n$, we now have a Fourier series in place of the Fourier integral (3.4):

$$[\mathcal{F}\psi](b) = \frac{1}{2\sqrt{\pi}} \sum_{\mathcal{L}_0\setminus\{0\}} |v|^{-\frac{1}{2}}\,\psi(v)\,e^{\frac{i}{2}vb}, \tag{4.6}$$

where the point $v = 0$ was removed from the transform because the state with support just at $v = 0$ is dynamically decoupled from the orthogonal sub-space spanned by states which vanish at $v = 0$. Since ψ are supported on $\mathcal{L}_0$, their images $\mathcal{F}\psi$ are periodic in b with the period π. Therefore one can restrict the support of the wave functions $[\mathcal{F}\psi](b)$ just to the circle $b \in [0, \pi]$, with the identification $[\mathcal{F}\psi](0) = [\mathcal{F}\psi](\pi)$.

By inspection, the elementary operators $\hat{v}$ and $\hat{\mathcal{N}}_\mu$ defined by

$$\hat{v}|v\rangle = v|v\rangle, \qquad \text{and} \qquad \hat{\mathcal{N}}_\mu|v\rangle = |v+\mu\rangle, \tag{4.7}$$

in the v representation are transformed to

$$\hat{v} = 2i\partial_b, \qquad \text{and} \qquad \mathcal{N}_\mu = e^{-i\mu b/2}. \tag{4.8}$$

in the b representation. As a consequence, the operator Θ_Λ assumes the form

$$\Theta_\Lambda = -12\pi G \left[(\sin(b)\partial_b)^2 - b_o^2 \partial_b^2 \right], \tag{4.9}$$

in the b representation, where, as before $b_o := \gamma\lambda\sqrt{\Lambda/3}$.

Let us first consider the case when $b_o \geq 1$ or $\Lambda \geq \Lambda_c := 3/\gamma^2\lambda^2$. In this case, Θ_Λ is essentially self-adjoint, whence one can readily repeat the procedure of section III C to construct the physical Hilbert space. However, because this Θ_Λ is negative, the physical Hilbert space is now zero dimensional! (For proofs, see [18].) Thus, in striking contrast to the WDW theory, in LQC a non-trivial quantum theory exists *only when the cosmological constant* Λ *is less than a critical value,* Λ_c. Because Λ_c, being of Planck scale, is approximately 10^{120} times the observed value of the cosmological constant, the constraint $\Lambda < \Lambda_c$ is not of phenomenological interest. Nonetheless, the fact that the cosmological constant has an upper bound in LQC is conceptually interesting. In the rest of this section, then, we will work with $\Lambda < \Lambda_c$.

B. Properties of Θ_Λ

1. *Weak solutions to the eigenvalue equation*

Note that, in the b-representation, the gravitational part of the Hamiltonian constraint is a differential operator as in the WDW theory. This suggests that one may be able to simplify it by a change of variables. We will now show that Θ_Λ can in fact be transformed to the *same* form as in the WDW theory:

$$\Theta_\Lambda = 12\pi G \, \mathrm{sgn}(|x| - x_o) \, \partial_x^2 \,. \tag{4.10}$$

However, there are two key differences. First, now the new variable takes values on a compact interval $x \in [-x_M, x_M]$, with points $-x_M$ and x_M identified. Second, the transformation is much more complicated in that x is defined in terms of the elliptic integral of the first kind $F(y,k)$:

$$x := \begin{cases} \frac{1}{\sqrt{1-b_o^2}} \, F(b',\, 1/(1-b_o^2)), & |b'| < B_o, \\ x_M - \frac{1}{b_o} F(\pi/2 - b', 1/b_o^2), & b' > B_o, \\ -x_M + \frac{1}{b_o} F(\pi/2 + b', 1/c^2), & b' < -B_o, \end{cases} \tag{4.11}$$

where

$$b' := b - \pi/2, \qquad B_o := \arcsin(b_o)$$
$$x_o := \frac{1}{\sqrt{1-b_o^2}} F(\pi/2 - B_o,\, 1/(1-b_o^2)), \qquad x_M := x_o + \frac{1}{b_o} F(B_o,\, 1/b_o^2) \,. \tag{4.12}$$

The dependence of x_o and x_M on b_o is shown in Fig. 3. In particular

$$\lim_{b_o \to 0} x_o(b_o) = +\infty, \qquad \lim_{b_o \to 0} [x_M - x_o](b_o) = \pi/2, \tag{4.13a}$$
$$\lim_{b_o \to 1} x_o(b_o) = \pi/2, \qquad \lim_{b_o \to 1} [x_M - x_o](b_o) = +\infty. \tag{4.13b}$$

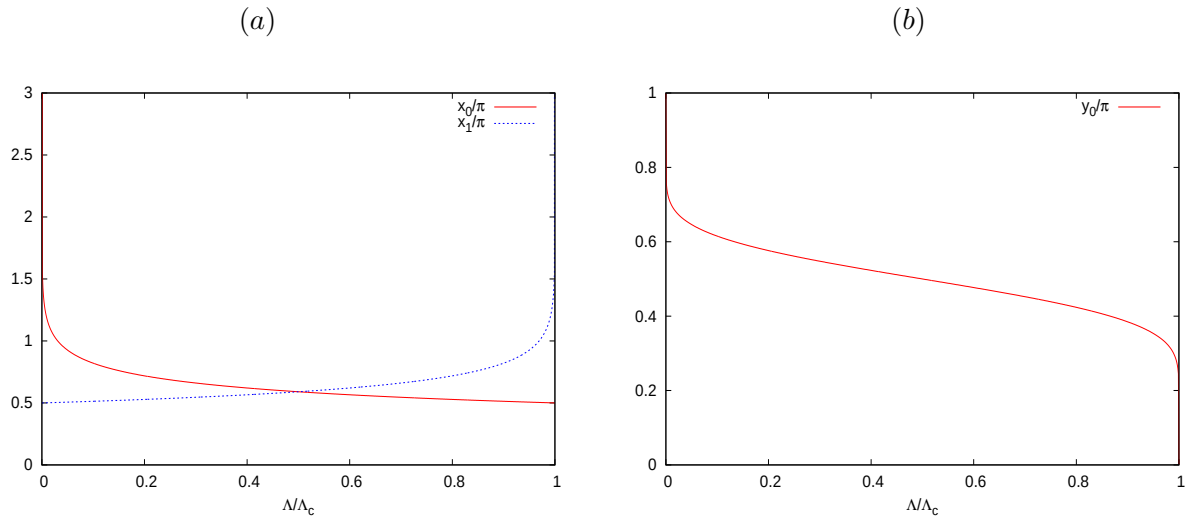

FIG. 3: (a) The dependence of the functions x_o and $x_1 := x_M - x_o$ (of (4.12)) on the cosmological constant Λ. (b) The dependence of $y_o = \pi x_o/x_M$ on Λ. Here $\Lambda_c = 3/\gamma^2\lambda^2$ is the critical value of Λ at which the energy density in the cosmological constant equals the maximum energy density $\rho_{\rm max}$ allowed by LQC in this model.

For the technical simplicity, it is convenient to introduce the rescaled variable

$$y := \pi \frac{x}{x_M} \quad \in [-\pi, \pi], \tag{4.14}$$

in terms of which the operator Θ_Λ takes the form

$$\Theta_\Lambda = \frac{12\pi^3 G}{x_M^2}\, \Theta'_\Lambda, \quad \text{where} \quad \Theta'_\Lambda := \mathrm{sgn}(|y| - y_o)\, \partial_y^2, \tag{4.15}$$

with $y_o := \pi x_o/x_M$.

We are now ready to analyze weak eigenfunction ψ_ζ of Θ'_Λ. As in the WDW analysis we will have to go back and forth between the v and the y representations. The weak eigenfunctions are distributional solutions to

$$(\psi_\zeta|\Theta'^\dagger \,-\, \bar{\zeta}\mathbb{I}\,|\chi\rangle = 0 \qquad \forall \chi \in \mathcal{D}\ , \tag{4.16}$$

where $\mathcal{D}$ now consists of states $\chi \in \mathcal{H}_{\rm gr}$ which have support only on a finite number of points of the lattice $\mathcal{L}$ on the v-axis. The particular form of the coefficients $f_{o,\pm}$ of Θ_o in Eq. (4.5) and the form of the inner product of $\mathcal{H}_{\rm gr}$ in the v-representation allows one to split each such eigenfunction ψ_ζ into components $\psi^\pm_\zeta$

$$\psi^\pm_\zeta(v) := \theta(\pm v)\, \psi_\zeta(v), \tag{4.17}$$

which again satisfy (4.16) as in the WDW theory. Secondly, as a function of y, any solution to (4.16) is necessarily of the form

$$\psi_\zeta(y) \;=\; \begin{cases} A(e^{i\sqrt{\zeta}y} + e^{-i\sqrt{\zeta}y}), & |y| \in [0, y_o) \\ B(e^{\sqrt{\zeta}(\pi-y)} + e^{-\sqrt{\zeta}(\pi-y)}), & |y| \in (y_o, \pi] \end{cases} \tag{4.18}$$

analogous to (3.12). These two observations allow us to directly apply the techniques developed in the final part of Sec. III A to find the necessary and sufficient conditions for (4.18) to satisfy (4.16). The result is a complete analog of the one in the WDW theory: the weak eigenfunctions have to be continuous in $y = \pm y_o$ but not necessarily differentiable there. This property transfers directly to the operator Θ_Λ for which any (weak) eigenfunction is again globally continuous, but not necessarily differentiable with respect to x at $x = \pm x_o$.

2. The self-adjoint extensions of Θ_Λ

We know already from the analysis of [18] that Θ_Λ admits a one parameter family of self-adjoint extensions, labeled by elements of $U(1)$. Each extension corresponds to particular asymptotic behavior of the basis functions $e(v)$ in the limit $v \to \infty$. Recall, however, that in the WDW theory, b-representation allowed us to find a more useful interpretation of the choice of extension in terms of gluing conditions at $b = \pm b_o$. The similarity of the WDW and LQC constraint operators and form of the eigenfunctions when expressed in terms of x variables (introduced respectively via (3.9) and (4.11)) suggests that a similar interpretation should exist also in LQC. We will now show that this expectation is correct.

For simplicity we again consider the operator Θ'_Λ. Its deficiency functions $\psi^\pm \in \mathcal{K}^\pm$ are the weak solutions to the equation (4.16) with the eigenfunctions $\zeta = \pm i$. Because of symmetry and the global continuity are of the form

$$\psi^\pm(y) = C \begin{cases} (1/c_+)(e^{(1\mp i)y/\sqrt{2}} + e^{-(1\mp i)y/\sqrt{2}}), & |y| < y_o, \\ (1/c_-)(e^{(1\pm i)(\pi-y)/\sqrt{2}} + e^{-(1\pm i)(\pi-y)/\sqrt{2}}) & |y| > y_o, \end{cases} \tag{4.19}$$

where

$$c_+ = e^{(1\mp i)y_o/\sqrt{2}} + e^{-(1\mp i)y_o/\sqrt{2}}, \tag{4.20a}$$

$$c_- = e^{(1\pm i)(\pi-y_o)/\sqrt{2}} + e^{-(1\pm i)(\pi-y_o)/\sqrt{2}}. \tag{4.20b}$$

Since all the eigenspaces are non-degenerate, there exists a 1-1 correspondence between these solutions and the appropriate eigenfunctions of Θ_Λ discussed in [18]. Since it was shown in [18] that all eigenfunctions of Θ_Λ are normalizable, it follows that eigenfunctions (4.19) are also normalizable. The unitary transformations between $\mathcal{K}^+$ and $\mathcal{K}^-$ and the extended domains are again given by the exact analogs of (3.18) and (3.19) respectively. The extension-characteristic terms ψ_α –analogs of (3.20)– are now of the form

$$\psi_\alpha(x) = C' \begin{cases} f(y, y_o, \alpha), & |y| < y_o, \\ f(\pi - y, \pi - y_o, -\alpha), & |y| > y_o, \end{cases} \tag{4.21}$$

where $C' \in \mathbb{C}$ and

$$f(y, y_o, \alpha) := \frac{1}{[\cosh(\sqrt{2}y_o) + \cos(\sqrt{2}y_o)]} \sum_{\rho,\sigma=\pm 1} e^{(y+\sigma y_o)\rho/\sqrt{2}} \cos\left[\frac{y - \sigma y_o}{\sqrt{2}} + \frac{\rho\alpha}{2}\right]. \tag{4.22}$$

Since $[\partial_x \psi](x = \pm x_o) = 0 \; \forall \psi \in \mathcal{D}$, the extensions are uniquely determined by the parameter β,

$$\beta(\alpha) := \arctan\left(\frac{[\partial_y^- \psi_a](y = y_o)}{[\partial_y^+ \psi_a](y = y_o)}\right) \in [0, \pi), \tag{4.23}$$

that encode the ratios between the left and right derivative of ψ_a at the gluing point $y = y_o$. With this parametrization, the choice of self-adjoint extensions can be directly interpreted in terms of gluing condition at $b = \pm b_o$ also in LQC. (Recall that in the classical theory, this is where the universe reaches the infinite volume.) Furthermore for any fixed value of $y_o \in]0, \pi[$ the function $\beta(\alpha)$ is a bijection of the circle of radius 1 onto the circle of radius 1/2. (See Appendix A for a proof of this assertion). Therefore, as in the WDW case, β is a convenient label for the extensions, equivalent to α, and Eq. (4.23) succinctly captures the domain $\mathcal{D}_\beta$ of $\Theta_{\Lambda,\beta}$. These properties will be used in the next subsection to identify the spectra of particular extensions $\Theta_{\Lambda,\beta}$ and the corresponding eigenbases in the physical Hilbert spaces.

C. The LQC physical sectors.

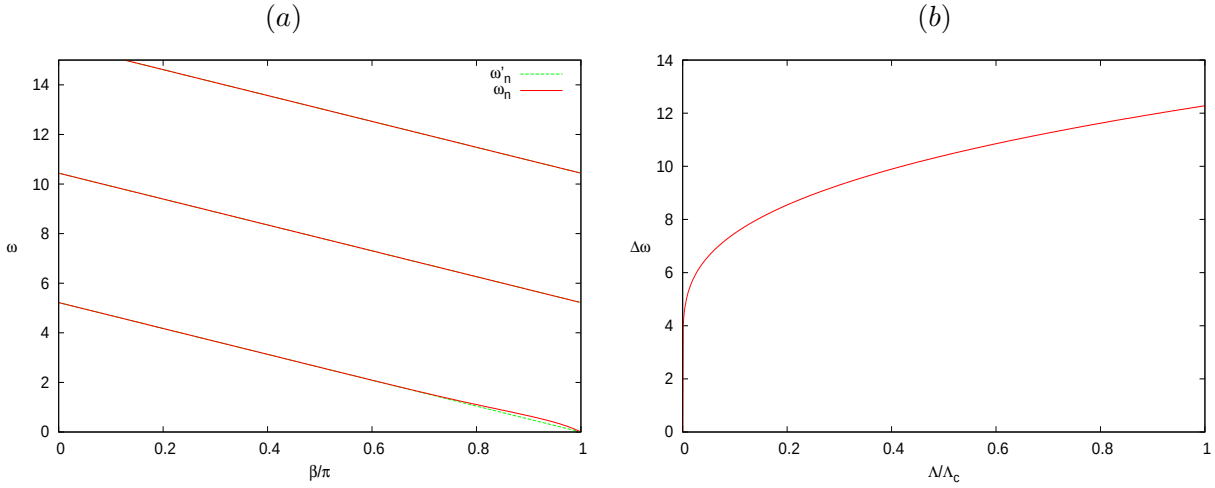

FIG. 4: (a) The lowest three eigenvalue ω_n are plotted as functions of the self-adjoint extension parameter β and compared with their approximations ω'_n obtained by neglecting the remnant $O(e^{-2\pi n(\pi-y_o)/y_o})$ in (4.27), for $\Lambda = 0.01\Lambda_c$. (b) the frequency gap $\Delta\omega$ is plotted as a function of cosmological constant.

We can now fix any one self-adjoint extension $\Theta_{\Lambda,\beta}$ of Θ_Λ in the quantum Hamiltonian constraint (4.3) and perform group averaging to obtain the physical Hilbert space $\mathcal{H}^{\rm phy}_\beta$. Because the spectra of $\Theta_{\Lambda,\beta}$ are discrete [18], the physical states are of the form

$$\Psi(x,\phi) = \sum_{n=0}^{\infty} \tilde{\Psi}_n \, e_{\beta,n}(x) \, e^{i\omega_{\beta,n}(\phi-\phi_o)}, \tag{4.24}$$

where the spectral profiles are square-summable sequences $\tilde{\Psi}_n$, and $e_{\beta,n}$ are the normalized eigenfunctions of $\Theta_{\Lambda,\beta}$ (belonging to $\mathcal{D}_\beta$), with eigenvalues $\omega^2_{\beta,n}$. Alternately, $e_{\beta,n}$ are eigenfunctions of the operator $\Theta'_{\Lambda,\beta}$ with eigenvalues k_n^2, related to ω_n via $\omega_n = (\sqrt{12\pi G}\,\pi/x_M)\, k_n$. They satisfy Eq. (4.23) and their functional form is given by

$$e_{\beta,n}(x) = N_{\beta,n} \begin{cases} \cosh[k_n(\pi - y_o)]\, \cos(k_n y), & |y| < y_o, \\ \cos[k_n y_o]\, \cosh[k_n(\pi - y)], & |y| > y_o, \end{cases} \tag{4.25}$$

where $N_{\beta,n}$ is a normalization factor and the eigenvalues $k_{\beta,n}$ are determined by the condition

$$\tan(k_n y_o) + \tanh[k_n(\pi - y_o)]\, \tan(\beta) = 0. \tag{4.26}$$

The form of (4.26) implies, in particular, that the spectra of $\Theta_{\Lambda,\beta}$ for different values of β are *disjoint*. Furthermore the lowest non-negative eigenvalue $\omega^2_{\beta,0}$ is an invertible function of β, whence the physical Hilbert spaces $\mathcal{H}^{\rm phy}_\beta$ corresponding to each extension are in fact *different* subspaces of $\mathcal{H}_{\rm gr}$.

Although the eigenvalues k_n^2 are provided only implicitly, the relation (4.26) allows us to determine their asymptotic behavior for large n explicitly:

$$k_n = (n\pi - \beta)/y_o + O(e^{-2\pi n(\pi - y_o)/y_o}). \tag{4.27}$$

Consequently, as n grows, the distribution of k_n quickly approaches the uniform one with the separation $\Delta k = \pi/y_o$. This property transfers directly to Θ_Λ, where

$$\lim_{n\to\infty} [\omega_{n+1} - \omega_n] = \Delta\omega := \sqrt{12\pi G}\, \pi^2/x_o, \tag{4.28}$$

Although the distribution of lower frequencies is not quite uniform, it approaches uniformity extremely fast (see Fig. 4a), and the asymptotic separation $\Delta\omega$ depends only on the value of the cosmological constant (see Fig. 4b). In particular

$$\lim_{\Lambda\to 0} \Delta\omega = 0 \quad \text{and} \quad \lim_{\Lambda\to\Lambda_c} \Delta\omega = 2\pi\sqrt{12\pi G}. \tag{4.29}$$

The form of the quantum Hamiltonian constraint (4.3) and of the physical states (4.24) allows us again to use the scalar field as an internal time and regard the square root of the positive part of $\Theta_{\Lambda,\beta}$ as the generator of time evolution on the subspace $\mathcal{H}^{\rm phy}_\beta = P^+_\beta \mathcal{H}_{\rm gr}$ of $\mathcal{H}_{\rm gr}$:

$$\Psi(x,\phi_o) \;\mapsto\; \Psi(x,\phi) = e^{i(\phi-\phi_o)\sqrt{|\Theta_{\Lambda,\beta}|}}\, \Psi(x,\phi_o) \qquad \forall\ \Psi(x,\phi) \in P^+_\beta \mathcal{H}_{\rm gr}, \tag{4.30}$$

where, as before, P^+_β is a projection onto the positive part of the spectrum of $\Theta_{\Lambda,\beta}$.

To obtain the physical consequences of this evolution, we will use observables $|\hat\theta|_\phi$ and $\hat\rho_{\rm tot}|_\phi$ in exact analogy with Eqs. (3.35) and (3.37) of the WDW theory. However, in contrast to the WDW theory, we cannot define $|\hat b|_\phi$ since the operator ∂_v fails to exist in LQC; we can only define its bounded, periodic functions such as $\sin(\hat b)|_\phi$.

D. LQC dynamics

To facilitate comparison with the WDW theory, we will use states closely resembling the Gaussians used in Sec. III D peaked about large $\omega^\star$:

$$\tilde\Psi_n = e^{-\frac{(\omega_n - \omega^\star)^2}{2\sigma^2}}\; e^{-i\omega_n\phi^\star} \tag{4.31}$$

where $\phi^\star$ is given by (3.40). we can then repeat the procedure used in the WDW theory to carry out numerical simulations. Specifically, these computations were performed in the following steps:

(i) First, the spectrum $\mathrm{Sp}(\Theta_{\Lambda,\beta})$ was found from (4.26). In all cases considered, the approximation provided by the analytical expression (4.27) turned out to be excellent.

(ii) Given any eigenvalue in $\mathrm{Sp}(\Theta_{\Lambda,\beta})$ the corresponding eigenfunction $\psi_{\beta,n}(v)$ was found in the domain $v \in \{4n : \ n = 1 \ldots N_1\}$ by solving the iterative difference equation

$$\omega_n^2 \, \psi_{\beta,n}(v) = [\Theta_{\Lambda,\beta}\psi_{\beta,n}](v) \tag{4.32}$$

with initial data $\psi_{\beta,n}(v = 4) = (-1)^n$. In various simulations, N_1 ranged from 10^5 to 2.5×10^5. Using the expression (4.2) of the scalar product in the v-representation, the norm of $\psi_{\beta,n}(v)$ was calculated using a polynomial extrapolation. The normalized eigenfunctions $\bar{e}_{\beta,n}(v)$ were then used together with the profile coefficients $\tilde{\Psi}_n$ of Eq. (4.31) to obtain the physical state $\Psi(v, \phi)$ in the v-representation:

$$\Psi(v, \phi) = \sum_{n=0}^{\infty} \tilde{\Psi}_n \, \bar{e}_{\beta,n}(v) \, e^{i\omega_{\beta,n}(\phi-\phi_o)} \tag{4.33}$$

where the sum extends over those n for which $\omega_n \in [\omega^\star - 7\sigma, \omega^\star + 7\sigma]$. This state is defined on points $v \in \{4n : \ n = 1 \ldots N_1\}$ and is simply the transform of the state in Eq. (4.24) to the v-representation. A key difference between the WDW theory is that, once the eigenvalues are obtained using (4.26), we can work directly in the v representation because, unlike in the WDW theory, the LQC eigenfunctions $\bar{e}_{\beta,n}(v)$ in the v representation can be easily handled numerically. (Recall that in the WDW theory, the corresponding eigenfunctions are Bessel functions of imaginary order which are difficult to deal with numerically.)

(iii) Expectation values and dispersions of the relational Dirac observables, $|\hat{\theta}|_\phi$, $\hat{\rho}_{\rm tot}|_\phi$ were computed directly in the v representation using the expressions (4.7) of $\hat{v}$ and the shift operator $\hat{\mathcal{N}}_\mu$. In particular, when the operator $\hat{\rho}_{\rm tot}$ is factor ordered as in the WDW theory, it becomes a simple combination of the shift operators:

$$\hat{\rho}_{\rm tot} = \frac{3}{8\pi G\lambda^2\gamma^2} \widehat{[\sin(b)]}^2 \, . \tag{4.34}$$

Note that the expression has the same form as 3.37) in the WDW theory, but the WDW operator $\hat{b}^2$ is now replaced by the bounded operator $\widehat{\sin(b)}^2$.

As in the WDW theory, a large number of simulations were performed by varying parameters of the initial state and the self-adjoint extension used in quantum dynamics. Fig. 5 illustrates the results of a typical simulation. The qualitative behavior is the same as that in the $\Lambda < 0$ case [8].

- States under consideration remain sharply peaked over a large number of 'epochs', where each 'epoch' is characterized as the evolution between consecutive quantum bounces. Thus, in each epoch the universe starts out with the maximum but finite total density $\rho_{\rm max}$, expands out till the matter density $\rho|_\phi$ vanishes and then recollapses, the density again reaching $\rho_{\rm max}$ at the end of the epoch.

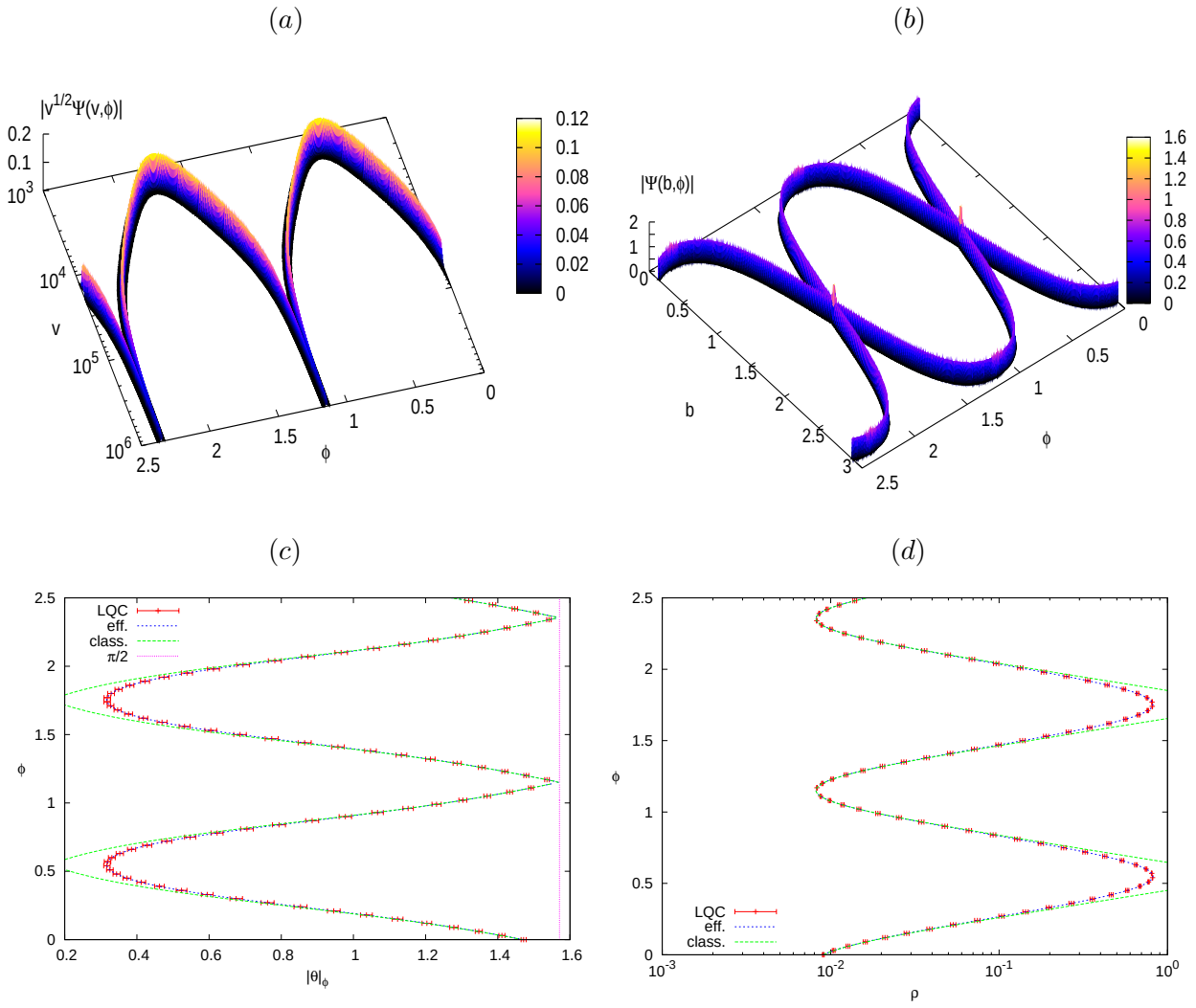

FIG. 5: LQC dynamics. Figures (a) and (b) show the evolution of the (absolute value of the) physical wave function in the v-ϕ and b-ϕ planes respectively. Figures (c) and (d) compare the expectation values of the Dirac observables $|\hat{\theta}|_\phi$ and $\hat{\rho}_{\rm tot}|_\phi$ with those in the effective and classical theories. Away from the Planck regime there is excellent agreement with (the analytical extensions of) solutions in general relativity. But in the Planck regime (left ends of figures (c) and (d)) there is a very large departure from the classical behavior because of quantum geometry effects. However, the effective trajectories capture the quantum evolution very well even in the Planck regime. In these simulations, the initial state was a gaussian peaked at $p^\star_\phi = 5 \times 10^3$ and $|\hat{\theta}|^\star_{\phi=0} = \arctan(10)$ with the relative spread $\Delta p_\phi/p_\phi = 0.03$. The self-adjoint extension corresponded to $\beta = 0$, the constant K in the definition of θ was set to $K = 5 \times 10^3$ and the cosmological constant was $\Lambda = 0.01\Lambda_c \approx 0.2\ell_{\rm Pl}^{-2}$.

- Expectation values of the Dirac observables $|\hat{\theta}|_\phi$ and $\hat{\rho}_{\rm tot}|_\phi$ are well approximated by the classical effective dynamics discussed in Appendix B *throughout* the evolution, including the quantum bounces. The difference between the two is much smaller than the dispersions of the corresponding Dirac observables.

- For $\Lambda \ll \Lambda_c := 3/\gamma^2\lambda^2$, quantum dynamics is well-approximated by the (analytically

extended) classical general relativity trajectory so long as the scalar field energy density is small compared to the Planck scale, $\rho|_\phi \ll \rho_{\rm Pl}$.

- However, as $\rho|_{\rm tot} = \rho|_\phi + \Lambda/(8\pi G)$ approaches the Planck scale, an effective repulsive force due to quantum geometry starts to dominate. It soon overwhelms the classical gravitational attraction and forces a quantum bounce at $\rho_{\rm tot} = \rho_{\rm max}$. As a result, the contracting quantum universe bounces back into an expanding quantum universe. As noted above, the wave functions remain sharply peaked even during the bounce and expectation values of Dirac observables follow those given by the effective equations even in the Planck regime.

- As in the WDW theory, quantum evolution is not unique because it depends on the choice of the self-adjoint extension $\Theta_{\Lambda,\beta}$ of Θ_Λ. Each extensions corresponding to the choice of a specific reflective boundary condition, but at $\rho_{\rm tot} = \Lambda/(8\pi G)$, and *not in the Planck regime near* $\rho_{\rm tot} \approx \rho_{\rm max}$.

- For any chosen self-adjoint extension, as in the WDW theory, the expanding universe recollapses after reaching zero matter density. However, unlike in the WDW theory, the big bang and the big crunch is replaced by quantum bounces. Therefore, we now have a nearly periodic evolution in LQC admitting an infinite chain of the bounces at the Planck energy density and recollapses at zero matter density The duration of each 'epoch' is given by
$$\Delta\phi \;\approx\; \frac{4y_o\Delta k}{\Delta\omega} \;\approx\; \frac{2x_o}{\sqrt{3\pi G}}. \tag{4.35}$$
to an excellent approximation.

- However, the distribution of ω_n is not exactly uniform. Consequently, quantum states slowly disperse from one cycle to the next. But for large ω_n deviations from uniformity decay much faster those in the case of $\Lambda < 0$ considered in [8]. Therefore the rate of dispersing is much slower than the already low rate found in [8].

- As in the WDW theory, the dependence on the choice of the self-adjoint extension is surprisingly weak for the states considered here. For generic states, results of the S-matrix discussion of [18] show that the dependence on β of expectation values of Dirac observables is negligible compared to the dispersion of the corresponding quantities. The dependence of dispersions on β is also very small compared to the dispersion $\delta_{\ln|k|}$ in the scalar field momentum (which is a constant of motion).

V. DISCUSSION

In this paper, we analyzed in detail the WDW theory and LQC of the k=0, $\Lambda > 0$ FLRW model along the lines of the treatment of the $\Lambda < 0$ case of [8], thereby completing the program outlined in an Appendix of [1]. As in the $\Lambda \leq 0$ cases, the scalar field can be used as a global clock, providing us with a natural notion of relational time both in the classical and quantum theories. However, interestingly, there is a key difference in the physically most interesting case, that of $\Lambda > 0$: In classical general relativity, solutions that start with infinite matter density ρ at the big bang at time $\phi = -\infty$ expand out and now achieve $\rho = 0$ at some *finite* value ϕ_o of internal time (when the volume v of the fiducial cell $\mathcal{C}$ becomes

infinite). Thus, in the ρ-ϕ plane each of these dynamical trajectories starts out at $\phi = -\infty$ but ends at $\phi = \phi_o$. But it can be *analytically* extended beyond $\phi = \phi_o$ and the extension represents a universe which starts out with zero matter density at $\phi = \phi_o$ but contracts, ending in a big crunch singularity at $\phi = \infty$. From the relational time perspective, then, one is led to regard the two branches as providing a single dynamical trajectory because it is artificial to simply end dynamics at a finite value of time. Now, in non-relativistic mechanics if the potential is negative and steep the particle may roll off to infinity in a finite amount of time. In that case, one has to choose from a one (or more) parameter family of boundary conditions at infinity to continue dynamics beyond that time. In the present case, by contrast, we did not have to resort to making a choice because the most interesting Dirac observable, $\rho|_\phi$, is analytic in ϕ.

Nonetheless, the fact that the universe expands out to $\rho = 0$ at a finite value of the relational time introduces ambiguities in the *quantum* evolution: The operator Θ_Λ which generates dynamics with respect to ϕ now fails to be essentially self-adjoint. Before discussing this point in detail, let us first note two aspects of this phenomenon. First, it is not a peculiarity of LQC; it occurs also in the WDW theory. Second, in both cases, the lack of essential self-adjointness is related directly with the behavior of the system at large v and low matter density ρ; its origin does *not* lie in the Planck scale physics. In both quantum theories, the dynamical operator admits a one parameter family of self-adjoint extensions. For a general system, different choices of extensions can give rise to very different dynamics. However, in this model the results are surprisingly robust with respect to this choice. Not only is the qualitative behavior of dynamics the same, but the differences in the dynamics of the expectation values of the most interesting Dirac observables in theories resulting from two different extensions are smaller than their dispersions in any one theory, even for general states. Furthermore, numerical simulations show that, irrespective of the choice of extension, quantum states which are semi-classical in the low curvature (or low total density $\rho_{\rm tot}$) regime remain sharply peaked at the *extended* classical trajectory in the low curvature regime both in the WDW theory and LQC. It is tempting to conjecture that this robustness of quantum dynamics is related to the fact that we did not have to choose a boundary condition at $\phi = \phi_o$ to extend the classical $\rho - \phi$ trajectory. In the remainder of this section, most of our discussion on the behavior of wave functions will refer to these states.

As in the $\Lambda \leq 0$ cases, there is a *pronounced* difference between the quantum dynamics of the two theories in the Planck regime. In the WDW theory, the wave function simply follows the extended classical trajectory into the big-bang and the big-crunch singularities. In LQC, by contrast, while these states remain peaked at the classical trajectory so long as the curvature (or $\rho_{\rm tot}$) is low compared to the Planck scale, there is a dramatic departure in the Planck regime. There is again a new repulsive force with origin in the quantum geometry that overwhelms classical gravity and cases a quantum bounce. Again, the numerical simulations show that, although the force is so strong in the Planck regime, it dies very quickly and becomes negligible once $\rho_{\rm tot}$ falls below $10^{-2} - 10^{-3}$ Planck density. In LQC then, even though we are in the k=0 case, we are led to a scenario that is approximately cyclic. As in the k=1 LQC models, the quantum evolution spans an infinite number of epochs. In each epoch the universe begins with a quantum bounce where $\rho_{\rm tot} \approx 0.41\rho_{\rm Pl}$, expands out till $\rho_{\rm tot} = \Lambda/8\pi G$ and then undergoes a collapse till it reaches another quantum bounce. For states under consideration, dynamics is nearly periodic.

How does this dynamics appear in the space-time picture? Let us begin with the classical

theory and consider a solution in which the universe starts out with a big-bang at $\phi = -\infty$. It expands out to $\mathcal{I}^+$ —which is space-like for $\Lambda > 0$— where the matter density vanishes and $\rho_{\rm tot} = \Lambda/8\pi G$. In terms of the physical metric, this space-time is future complete. However, the extended phase space trajectory analytically continues the space-time geometry across $\mathcal{I}^+$, effectively gluing it with $\mathcal{I}^-$ of a contracting solution.[6] Quantum states under consideration remain peaked at these extended space-time geometries across $\mathcal{I}$. An extension is but to be expected both in the WDW theory and in LQC: quantum evolution in the internal time ϕ is *unitary* and ϕ achieves a finite value ϕ_o at $\mathcal{I}$ of the given classical solution, unitary evolution could not just stop there. What is interesting is that, *irrespective of the choice of the self-adjoint extension*, the state remains sharply peaked on the analytically extended geometry.

This extension, and the ensuing nearly cyclic scenario has some similarities with Penrose's recent proposal of a cyclic conformal cosmology [24]. However, there are also key differences. In our case, $\mathcal{I}^+$ of the expanding branch is glued to the $\mathcal{I}^-$ of the contracting branch; not to the big-bang singularity of the next 'aeon'. More importantly, quantum geometry effects are crucial in LQC. In particular $\hbar$ appears in the denominator of the expression of the maximum density $\rho_{\rm max}$ whence, as one would expect, $\rho_{\rm max}$ would diverge in the classical limit $\hbar \to 0$. Therefore, quantum effects and a non-zero $\hbar$ play an essential role in the approximately cyclic scenario of LQC. By contrast, a central feature of the cyclic conformal cosmology paradigm is that, although one does have unboundedly large curvatures, $\hbar$ plays no role at all in this regime.

Use of the scalar field as a relational time variable played a key role throughout our analysis, both in the classical and quantum theory. What would have happened if we had made some other choice? In a recent analysis [25, 26] non-rotating dust has been used in place of the scalar field. In this case, the expression (4.3) of the gravitational part Θ_Λ of the Hamiltonian constraint is modified because the lapse is now tailored to proper time. In particular, the coefficient of Λ is now *linear* rather than *quadratic* in v. Consequently, the analog of Θ_Λ is now essentially self-adjoint and the LQC evolution resembles that in the $\Lambda = 0$ case [1]: The universe starts out with infinite volume in the distant past, collapses, undergoes a quantum bounce and then expands out to infinite volume. However, in the Planck regime, quantum matter should be described using quantum field theory and for all standard quantum fields the kinetic term in the Hamiltonian is quadratic in momenta. Therefore the specific feature that simplifies the mathematics in the case of dust is no longer available and the overall situation is then the same as that in the case of the scalar field.

But what if we return to using scalar field as matter source but let a geometric variable be the relational time? An obvious choice is volume. But in LQC, volume fails to be single valued making it difficult to introduce the 'time-dependent' relational Dirac observables —such as the matter density operator $\hat{\rho}|_v$— especially near the bounce. On the other hand, the conjugate variable b is single valued both on classical and effective trajectories and, as the form of the Hamiltonian constraint suggests, the function y it determines is a possible candidate for relational time. However, it appears that the evolution would then be unambiguously unitary only for $|y| > y_o$. Furthermore, defining the physical state would require specification of the initial data at $y = y_o$ but the theory does not provide any

[6] The detailed gluing procedure will involve a conformal completion along the lines of [23] where the normal component to $\mathcal{I}$ of the metric is rescaled by a different power of the conformal factor than the tangential one.

selection principle for this task. These difficulties with v and b could well be surmountable with new ideas and more careful analysis. But as of now they seem to be more serious handicaps than the complications associated with the use of the scalar field as relational time we encountered in this paper.

Could one perhaps retain scalar field as the matter source but set lapse $N = 1$ in the quantum constraint and use a 'timeless framework' in LQC? Results of [15, 27] imply that we would have been led to a theory that is mathematically free of ambiguities associated with self-adjoint extensions. However, as we now explain, this theory is difficult to interpret and it is unclear whether it is physically viable. We will conclude our discussion with a detailed elaboration of this point.

With lapse $N = 1$, the quantum Hamiltonian constraint has the form $\hat{C} = B(v) \otimes \partial_\phi^2 + \hat{C}_{\rm gr} \otimes \mathbb{I}$ where $C_{\rm gr}$ is the gravitational part of the Hamiltonian constraint and $B(v) \sim 1/v$ for large values of v (see, e.g., [1]). This total constraint operator $\hat{C}$ has been shown to be essentially self-adjoint [18] and for simplicity we will denote its self-adjoint extension also by $\hat{C}$. One can therefore use it directly for group averaging and construct the physical Hilbert space $\mathcal{H}^{\rm phy}$ in the 'timeless framework' without recourse to deparametrization. Then, although states can be represented as wave functions $\Psi(v, \phi)$, the physical scalar product is no longer given by an integral over v at a fixed value of ϕ. What is the relation between this $\mathcal{H}^{\rm phy}$ and the Hilbert spaces $\mathcal{H}^{\rm phy}_\beta$ associated with self-adjoint extensions $\Theta_{\Lambda,\beta}$ we constructed in this paper? It turns out [27] that $\mathcal{H}^{\rm phy}$ is huge; it is given by the *direct integral* of all $\mathcal{H}^{\rm phy}_\beta$; $\mathcal{H}^{\rm phy} = \int_{\oplus\, I} \mathcal{H}^{\rm phy}_\beta \, {\rm d}\beta$, where I is the interval $(0, \pi)$.

We will briefly discuss a simple example —due to Wojciech Kamiński in [28]— to illustrate the relation between these Hilbert spaces. Consider a 2-dimensional strip, $M = \mathbb{R} \times [0, 1]$, with coordinates $\phi \in \mathbb{R}$ and $x \in [0, 1]$ and a constraint thereon in the form of the Schrödinger equation $(-i\partial_\phi + i\partial_x)\Psi(x, \phi) = 0$ (with a first-order Hamiltonian). As in LQC, ϕ plays the role of time while x is to be thought of as the analog of the compactified volume coordinate θ. The operator $\Theta_x := -i\partial_x$ fails to be essentially self-adjoint on the closed interval $[0, 1]$; it admits a 1-parameter family of self-adjoint extensions $\Theta_{x,\beta}$, labeled by $\beta \in [0, 2\pi)$ (with domain $\mathcal{D}_\beta$ given by wave functions $\psi(x)$ satisfying $\psi(1) = e^{i\beta}\psi(0)$). For each extension, we can construct a physical Hilbert space $\mathcal{H}^{\rm phy}_\beta$ in the standard manner from solutions to the quantum constraint: $\Psi(x, \phi) \in \mathcal{H}^{\rm phy}_\beta$ if and only if $-i\partial_\phi \Psi(x, \phi) = \Theta_{x,\beta}\, \Psi(x, \phi)$. Next, let us define $\mathcal{H} := \int_{\oplus\, I} \mathcal{H}^{\rm phy}_\beta \, {\rm d}\beta$, with $I = (0, 2\pi)$. ($\mathcal{H}$ is analogous to $\mathcal{H}^{\rm phy}$ obtained by group averaging in [27]). Every $\Psi_\beta(x, \phi) \in \mathcal{H}^{\rm phy}_\beta$ can be expanded as

$$\Psi_\beta(x, \phi) = \sum_{n=-\infty}^{\infty} \tilde{\psi}_{\beta,n}\; e^{i(2\pi n+\beta)x}\; e^{ik\phi} \tag{5.1}$$

where $k := 2\pi n + \beta$. On the other hand $\Psi(x, \phi) \in \mathcal{H}$ has the form

$$\begin{aligned} \Psi(x, \phi) &= \int_0^{2\pi} {\rm d}\beta\, \Psi_\beta(x, \phi) = \sum_{n=-\infty}^{\infty} \int_0^{2\pi} {\rm d}\beta\, \tilde{\psi}_{\beta,n}\, e^{i(2\pi n+\beta)x}\, e^{ik\phi} \\ &= \int_{-\infty}^{\infty} {\rm d}k\, \tilde{\Psi}(k)\, e^{ikx+ik\phi}\,, \end{aligned} \tag{5.2}$$

where we have set $k = 2\pi n + \beta$ as above. The norms in $\mathcal{H}^{\rm phy}$ are given by:

$$\|\Psi(x,\phi)\|^2 = \int_{-\infty}^{\infty} \mathrm{d}k\, |\tilde{\Psi}(k)|^2\,. \tag{5.3}$$

Note that $\tilde{\Psi}(k)$ has support on the entire k-axis and furthermore, the norm of $\Psi(x,\phi)$ also involves the integral of $|\tilde{\Psi}(k)|^2$ over the entire k axis. Therefore, while elements $\Psi_\beta(x,\phi)$ of any one $\mathcal{H}^{\rm phy}_\beta$ are restricted to have support only on the physical configuration space $M = \mathbb{R}\times[0,1]$, $\Psi(x,\phi)$ in $\mathcal{H}^{\rm phy}$ are allowed to be non-zero all along the x-axis, even though points outside the x-interval $[0,1]$ have no physical interpretation in the model under consideration. In other words, although we restricted ourselves only to a 'strip' $M = \mathbb{R}\times[0,1]$ of the Minkowski space in defining the classical system, in effect $\mathcal{H}^{\rm phy}$ describes a system on the entire 2-dimensional Minkowski space $\mathbb{R}^2$. [7] To summarize, for the particle on the strip M, one would physically expect that the quantum theory should be formulated just on M since values of x outside $[0,1]$ have no physical meaning. This expectation is borne out if one works with any one self-adjoint extension $\Theta_{x,\beta}$ of Θ_x but not if one works with the direct integral $\mathcal{H}^{\rm phy}$ of all the resulting Hilbert spaces.

In LQC, the situation is analogous. Working with a specific self-adjoint extension allows us to remain in the interval $[0,\infty]$ of the $|v|$-axis, introduce Dirac observables and track their evolution in the internal time ϕ and compare it with classical trajectories. On the other hand, working in the timeless framework in effect requires us to extend the v-axis beyond $v=\infty$ and this extension is difficult to interpret physically.[8] For the same reason, while one can introduce Dirac observables also in the timeless framework, we cannot ask for their 'evolution' and it is difficult to compare predictions of the quantum theory with those of the classical. In particular, while the choice $N=1$ of the lapse yields evolution in proper time in the classical theory, unfortunately this interpretation does not extend to the quantum theory in a simple way. Thus, while at first it seems mathematically natural to work with the lapse $N=1$ because the full constraint is then essentially self-adjoint, the resulting Hilbert space $\mathcal{H}^{\rm phy}$ appears to be simply too large to be physically viable in the above context.

Finally, our analysis brought out an unexpected robustness of the quantum evolution with respect to the choice of self-adjoint extensions $\Theta_{\Lambda,\beta}$. As we noted above, this may be related to the fact that, in the physical sector associated with *any* self-adjoint extension, under unitary evolution quantum states of interest follow the natural and unambiguous analytic extension of classical trajectories. Is this perhaps a special case of as yet unknown general result? Is the lack of sensitivity of the quantum evolution on the choice of analytic extensions have its origin in some special features of the classical evolution?

Acknowledgments

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[7] Note that, since the basis functions $e^{i(2\pi n+\beta)x}$ can be extended analytically to the entire x-axis, the quantum constraint can be uniquely extended to the full Minkowski space $\mathbb{R}^2$.

[8] Furthermore, unlike in the simple example discussed above, here one cannot extend the constraint operator uniquely even if one expresses the basis vectors as functions of the 'compactified volume' coordinate θ of (3.34), as these functions are not analytic in $\theta = \pi/2$.

Natural Sciences and Engineering Research Council of Canada. The numerical analysis has been performed with use of the numerical LQC library presently developed by T. Pawłowski and J. Olmedo.

Appendix A: Bijectivity of $\beta(\alpha)$

In section IV B we began by labeling the self-adjoint extensions of Θ_Λ by a parameter α and then switched to a more convenient parameter β. In this appendix, we will show that the map $\alpha \to \beta$ is bijective, i.e. that the β parametrization used to denote self-adjoint extensions as $\theta_{\Lambda,\beta}$ is viable.

The definition of β and the periodicity $\beta(\alpha) = \beta(\alpha+\pi)$ —a direct consequence of its form given by (4.21), (4.22) and (4.23)— imply that $\beta(\alpha)$ is a well defined continuous function mapping from a circle of radius 1 to a circle of radius 1/2. Therefore to establish the desired bijective property it suffices to prove that, for any given $y_o \in]0, \pi[$, the derivative of β with respect to α is bounded and isolated from zero.

Let us consider first the function $X(y_o, \alpha) := \tan(\beta)$ which can be decomposed as follows

$$X(y_o, \alpha) = \frac{f_1(y_o) g_1(y_o, \alpha)}{f_2(y_o) g_2(y_o, \alpha)}, \tag{A1}$$

where

$$f_1 = \cosh(\sqrt{2}(\pi - y_o)) + \cos(\sqrt{2}(\pi - y_o)), \tag{A2a}$$
$$f_2 = \cosh(\sqrt{2} y_o) + \cos(\sqrt{2} y_o), \tag{A2b}$$

and

$$\begin{aligned} g_1 = {} & \sinh(\sqrt{2} y_o)[\cos(\alpha/2) - \sin(\alpha/2)] \\ & - \sin(\sqrt{2} y_o)[\cos(\alpha/2) + \sin(\alpha/2)], \end{aligned} \tag{A3a}$$

$$\begin{aligned} g_2 = {} & \sinh(\sqrt{2}(\pi - y_o))[\cos(\alpha/2) + \sin(\alpha/2)] \\ & + \sin(\alpha/2 - \sqrt{2}(\pi - y_o)). \end{aligned} \tag{A3b}$$

It is straightforward to check by inspection, that both f_1 and f_3 are strictly positive and isolated from 0.

The derivative of X over α takes the form

$$X'(y_o, \alpha) = \frac{f_1(y_o) f_3(y_o)}{2 f_2(y_o) g_2^2(y_o, \alpha)}, \tag{A4}$$

where the function

$$\begin{aligned} f_3 = {} & \cosh(\sqrt{2}(\pi - 2y_o)) - \cosh(\sqrt{2}\pi) \\ & + \cos(\sqrt{2}(\pi - y_o)) \sin(\sqrt{2} y_o) - \sinh(\sqrt{2} y_o) \\ & + \sin(\sqrt{2}(\pi - y_o)) \sin(\sqrt{2} y_o) + \sinh(\sqrt{2} y_o) \end{aligned} \tag{A5}$$

has (also by inspection) the following properties

- $f_3(y_o = 0) = 0$,

- $\forall y_o \in [10^{-3}, \pi]$ $f_3(y_o) \in [-50, -0.1]$,
- $\forall y_o \in [0, 10^{-3}]$ $[\partial_{y_o} f_3](y_o) \in [-123.0, -122.5]$,

which again implies its boundedness and isolation from zero for any $0 < y_o < \pi$.

The derivative $\partial_\alpha \beta$ can be expressed using X, X' as follows:

$$[\partial_\alpha \beta](\alpha, y_o) = \frac{X'(y_o, \alpha)}{1 + X^2(y_o, \alpha)} = \frac{f_1 f_2 f_3}{f_1^2 g_1^2 + f_2^2 g_2^2} \tag{A6}$$

and by the properties of f_1, f_2, f_3 it never vanishes and can reach infinity only when both g_1 and g_2 vanish simultaneously. The condition $g_1 = g_2 = 0$ can be reexpressed as the linear system of equations for $\sin(\alpha/2)$ and $\cos(\alpha/2)$ (treated as independent variables). The existence of the nontrivial solution to that system requires that the determinant of the equation matrix vanishes, that is

$$\begin{aligned}[\sinh(\sqrt{2}(\pi - y_o)) + \cos(\sqrt{2}(\pi - y_o))] \times [\sinh(\sqrt{2} y_o) - \sin(\sqrt{2} y_o)] \\ + [\sinh(\sqrt{2} y_o) + \sin(\sqrt{2} y_o)] \times [\sinh(\sqrt{2}(\pi - y_o)) - \sin(\sqrt{2}(\pi - y_o))] = 0.\end{aligned} \tag{A7}$$

Since all the terms in the square brackets are explicitly positive within $y_o \in]0, \pi[$ this condition is never satisfied. Therefore, the denominator of the rightmost expression in (A6) never vanishes, so for fixed value of y_o the derivative $\partial_\alpha \beta$ is bounded due to the continuity of X, X' and the compactness of the domain of α. Thus we have

$$0 > c \geq [\partial_\alpha \beta](y_o, \alpha) \geq C > -\infty. \tag{A8}$$

Appendix B: Classical effective dynamics

In Sec. IV D we found that wave functions which start out being sharply peaked on a classical trajectory in the low curvature region remain sharply peaked throughout the evolution, including the Planck regime. This strongly suggests that there may be effective dynamical trajectories on the classical phase space which incorporate the appropriate quantum corrections in the Planck regime and approximate the full quantum evolution quite well throughout evolution. A particularly convenient heuristic method to arrive at these effective equations was proposed in [29] and later derived more systematically analytically in the case $\Lambda = 0$ [30]. It was successfully tested in several cases of isotropic LQC [1, 8, 9, 31]. Here we briefly recall how these effective equations arise by adapting the detailed discussion for the $\Lambda < 0$ model from [8] to the $\Lambda > 0$ case now under consideration.

The strategy comes from a geometrical formulation of quantum mechanics in which the quantum Hilbert space is regarded as an infinite dimensional symplectic manifold, sometimes called 'the quantum phase space'. The idea is to find an embedding of the finite dimensional classical phase space into this infinite dimensional 'quantum phase space' such that the full quantum evolution preserves the image of the embedding to a good approximation. For a harmonic oscillator, the embedding is provided by coherent states (whose dispersions are determined by the mass and the spring constant). Such an embedding is possible also for FLRW models [30, 32](for a brief summary, see [4]). The result is a quantum corrected, effective constraint. Although it is simply a function on the classical phase space —obtained by taking the expectation values of the quantum constraint operator in states corresponding

to the image of the embedding— it differs from the classical constraint function by terms involving $\hbar$. As mentioned above, dynamical trajectories generated by this effective Hamiltonian constraint have turned out to provide an excellent approximation to the full quantum evolution of states that start out to be sharply peaked around a classical trajectory in the low curvature regime.

In the LQC literature, the effective Hamiltonian constraint is written using lapse $N = 1$ so that it generates evolution in proper or cosmic time. Therefore, to facilitate comparison, we will do the same here. Then, the effective Hamiltonian constraint is given by

$$\mathcal{H}_{\rm eff} = -\frac{3}{8\pi G\gamma^2\bar{\mu}^2}\,|p|^{\frac{1}{2}}\,\sin^2(\bar{\mu}c) \,+\, \frac{1}{2}\frac{p_{(\phi)}^2}{|p|^{\frac{3}{2}}} \,+\, \frac{p^{\frac{3}{2}}}{8\pi G}\,\Lambda \approx 0\,. \tag{B1}$$

By calculating the Hamilton's equations from $\mathcal{H}_{\rm eff}$, and using (B1) again to simplify the resulting expressions, one arrives to the following evolution equation for the energy density ρ of the scalar field:

$$\rho' = \pm\, 4\sqrt{3\pi G}\left[\rho\,\rho_{\rm tot}\left(1 - \frac{\rho_{\rm tot}}{\rho_{\rm max}}\right)\right]^{1/2}. \tag{B2}$$

where $\rho_{\rm tot} := \rho + \Lambda/(8\pi G)$ and the prime denotes the derivative with respect to the scalar field ϕ. (Thus, one first calculates the derivatives of p and ϕ with respect to proper time by taking Poisson brackets of p and ϕ with $\mathcal{H}_{\rm eff}$ and then combines them to find p' and then ρ'.) However this equation is inconvenient to use in numerical simulations because it is not regular at $\rho = 0$ and $\rho_{\rm tot} = \rho_{\rm max}$. Also, the sign in front of the righthand side changes in the process of evolution (at the bounce where $\rho_{\rm tot} = \rho_{\rm max}$ and at the recollapse where $\rho = 0$). Therefore for the purpose of finding the solution it is more convenient to use the second order equation derived from (B2),

$$\rho'' = 24\pi G\left[(2\rho + \rho_{\rm tot})\left(1 - \frac{\rho_{\rm tot}}{\rho_c}\right) - \rho\right], \tag{B3}$$

which admits a unique global solution to the initial value problem with the initial data $(\rho(\phi_o), \rho'(\phi_o))$, where $\rho'(\phi_o)$ is determined from $\rho_{\rm tot}$ via (B2).

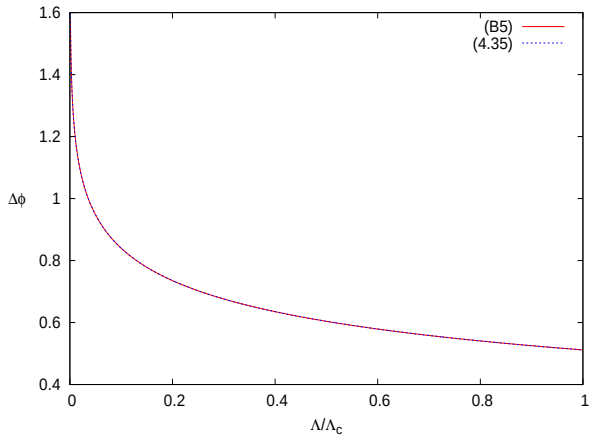

FIG. 6: The period $\Delta\phi$ of the evolution predicted by the effective theory via (B4) is compared against the approximate period of the genuine quantum evolution (4.35).

This equation have been solved analytically [33]. But the solution is expressed in terms of elliptic integrals of the first and second kind whose values have to be found numerically. Therefore, here it is more convenient to solve it numerically from the beginning. In the actual calculations (such as the ones presented in Fig. 5) this step was carried out with the use of the adaptive Runge-Kutta method of the 5th order known as *RK45* (Cash-Carp).

The form of equation (B3) implies already that the trajectory $\rho(\phi)$ is periodic, with the period given by a direct integration of (B2):

$$\Delta\phi = \frac{1}{\sqrt{12\pi G}} \int_{\rho=0}^{\rho_{\rm tot}=\rho_c} \mathrm{d}\rho \left[\rho_{\rm tot}\,\rho\left(1-\frac{\rho_{\rm tot}}{\rho_c}\right)\right]^{-1/2}. \tag{B4}$$

The dependence of $\Delta\phi$ on the value of cosmological constant is presented in Fig. 6, where its values were calculated numerically via the standard trapezoid method. The extremal points correspond respectively to the values $\rho = 0$ (minimum corresponding to the recollapse at infinite volume) and $\rho = \rho_{\rm max} - \Lambda/(8\pi G)$ (maximum corresponding to the quantum bounce).

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