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Robustness of key features of loop quantum cosmology

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Abstract

Loop quantum cosmology of the $k=0$ FRW model (with a massless scalar field) is shown to be exactly soluble if the scalar field is used as the internal time already in the classical Hamiltonian theory. Analytical methods are then used i) to show that the quantum bounce is generic; ii) to establish that the matter density has an absolute upper bound which, furthermore, equals the critical density that first emerged in numerical simulations and effective equations; iii) to bring out the precise sense in which the Wheeler DeWitt theory approximates loop quantum cosmology and the sense in which this approximation fails; and iv) to show that discreteness underlying LQC is fundamental. Finally, the model is compared to analogous discussions in the literature and it is pointed out that some of their expectations do not survive a more careful examination. An effort has been made to make the underlying structure transparent also to those who are not familiar with details of loop quantum gravity.

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I. INTRODUCTION

The status of loop quantum cosmology (LQC) of FRW models has evolved significantly over the last year. Specifically, when there is at least one massless scalar field present, the *physical* sector of the theory was constructed in detail and then used to show that the big bang is replaced by a quantum bounce. Furthermore, this singularity resolution does not come at the cost of introducing undesirable features such as unphysical matter or large quantum effects in physically tame situations. We will begin with a brief summary of these results particularly because there is some confusion in the literature on the bounce scenario and on the difference between LQC and the Wheeler DeWitt (WDW) theory.

In these LQC models, the availability of the physical inner product on the space of solutions to the Hamiltonian constraint and of a complete set of convenient Dirac observables led to a precise construction of suitable semi-classical states. Numerical evolution of these states then led to a number of detailed and quantitative results: i) Classical general relativity is an excellent approximation to quantum theory until matter density reaches $\sim 0.01\rho_{\text{Pl}}$, or, scalar curvature reaches $\sim -0.15\pi/\ell_{\text{Pl}}^2$; ii) As curvature increases further, quantum geometry becomes dominant, creating an effective repulsive force which rises very quickly, overwhelms classical gravitational attraction, and causes a bounce at¹ $\rho \sim 0.41\rho_{\text{Pl}}$, thereby resolving the classical singularity. The repulsive force dies very quickly once the density falls below $0.41\rho_{\text{Pl}}$; iii) While the classical evolution breaks down at the singularity, the full quantum evolution remains well defined, joining the pre-big-bang branch of the universe to the post-big-bang branch through a *deterministic* evolution; and, iv) Contrary to the earlier belief, the so-called ‘inverse volume effects’ associated with the matter Hamiltonian are inessential to the singularity resolution in these models. At the Planck scale, dynamics of semi-classical states is dictated, rather, by the quantum geometry effects in the *gravitational part* of the Hamiltonian constraint. (For details, see, e.g., [1–4, 6, 7].)

These results also addressed two concrete criticisms [8, 9] of the earlier status of LQC. First, although it had been demonstrated [10] that the quantum Hamiltonian constraint remains well-defined at the putative singularity, in absence of a physical inner product and Dirac observables the physical meaning of this singularity resolution had remained unclear. One could therefore ask [8]: What is the precise and physically relevant sense in which the singularity is resolved? Second, while the early formulations of the quantum Hamiltonian constraint [10, 11] were an improvement over the Wheeler-DeWitt (WDW) theory near the singularity, they turned out to have a serious flaw: they could lead to a significant deviation from classical general relativity even in regimes in which the space-time curvature is quite low [2]. In particular, in the $k=0$ model, more the state is semi-classical, lower was the matter density and curvature at which the bounce occurred [2, 3]. In particular, for perfectly reasonable semi-classical states, the bounce could occur even at density of water! In presence of a cosmological constant, serious deviations from classical general relativity also occurred in low curvature regions well away from the singularity. These problems can also occur without a cosmological constant. As a result, in the $k=1$ model it was then natural

¹ In early papers (e.g., [1–4]) the bounce was said to occur at $\rho = 0.82\rho_{\text{Pl}}$. However to calculate the quantum Hamiltonian constraint these papers used the lowest non-zero eigenvalue of the area operator for the area gap. It was later realized that the corresponding eigenstates are not suitable for homogeneous cosmologies. On the space of states which *are* suitable, the area gap is twice as large, which makes the critical density half as large [5].

to ask [9]: does LQC predict that there would be a recollapse from the expanding to the contracting phase that can occur at low curvatures in classical general relativity? Absence of recollapse would be an unacceptable, *qualitative* departure from general relativity.

Because the physical sector of the theory has now been constructed in detail, both these issues could be addressed satisfactorily [3, 4, 6]. First, ‘singularity resolution’ refers to the behavior of Dirac observables such as matter density, whence the physical meaning of the term is now transparent. Second, not only is there a recollapse in the $k=1$ model but there is excellent *quantitative* agreement with general relativity (for universes which grow to macroscopic sizes) [4]. These investigations have also shown that, while the singularity can be removed rather easily in LQC, considerable care is needed in the formulation of quantum dynamics to ensure that the detailed predictions do not lead to gross departures from classical general relativity in tame situations [2, 3]. Careful treatment ensures both a good ultra-violet behavior (singularity resolution) *and* a good infra-red behavior (agreement with general relativity at low curvatures) [3, 4]. In particular, in the ‘improved’ LQC dynamics [3, 4], the quantum bounce occurs only when the matter density is $\sim 0.41\rho_{\text{pl}}$, irrespective of the choice of semi-classical states. Once the curvature is low, evolution is close to that predicted by classical general relativity also in the presence of a cosmological constant [3].²

However, even within the confines of these simple models, a number of questions still remain. First, numerical simulations and effective equations both imply that the bounce occurs when the matter density reaches a critical value $\rho_{\text{crit}} \approx 0.41\rho_{\text{pl}}$. It turned out that ρ_{crit} is insensitive to the sign or value of the cosmological constant and is the same whether we consider $k=0$ or $k=\pm 1$ models [3, 4, 14]. Can one understand the physical origin of ρ_{crit} ? Is there an upper bound on matter density in physical quantum states which can be established without having to make the assumptions that underlie numerical simulations and effective equations? Second, the detailed evolution was restricted to states which are semi-classical at late times and was carried out numerically. Therefore, an analytical understanding of quantum evolution has been lacking and, in particular, the precise reason for the striking differences between LQC and the WDW theory has not been fully understood. While states which are semi-classical at late times are the most interesting ones, are they essential for the bounce scenario as some authors have suggested? Or, is there a sense in which all states undergo a quantum bounce? It has been suggested [15] that the near symmetry (in intrinsic time) of volume uncertainties around the bounce point is a consequence of the use of a special class of semi-classical states at late times. Is this the case or is it shared by a much more general class of states which are (truly) semi-classical at late times?

Similarly, comparison of LQC and the WDW theory raises a number of questions. There is a precise sense [2, 3, 11] in which the quantum Hamiltonian constraint of the WDW theory approximates that of LQC. Yet, the physical content of the *solutions* to the two constraints is dramatically different: while none of the states of the WDW theory which are semi-classical at late times can escape the big bang singularity, all their analogs in LQC do just that. What then is the precise relation between the two sets of dynamics? Can one make statements

² These important differences between the improved dynamics (sometimes referred to as the $\bar{\mu}$ evolution) and the older one (referred to as the μ_o evolution) appear not to have been fully appreciated. Indeed, some of the recent discussions [12, 13] portray the two schemes as if they are on equal footing. As discussed in section VI, the issue of whether any of the proposed dynamics of LQC can be systematically derived from LQG is wide open but it is logically distinct from whether they are viable within the confines of LQC. Mixing of these two issues has resulted in some unfortunate confusion in the literature.

for more general states? While the geometric part of the WDW Hamiltonian constraint is a second order differential operator, that of LQC is a second order difference operator, the step size being dictated by the ‘area gap’ Δ , i.e., the smallest non-zero eigenvalue of the area operator. What happens in the mathematical limit in which Δ is sent to zero by hand? Non-relativistic quantum mechanical systems also admit a ‘polymer’ representation (of the Weyl algebra) which mimics the mathematical structure of loop quantum cosmology [16]. For a harmonic oscillator, dynamics in this representation involves a (mathematical) discreteness parameter ℓ and is distinct from the standard Schrödinger dynamics. However, as was shown in detail in [16–18], it reduces to the standard dynamics in the limit in which ℓ goes to zero. Is the situation similar in LQC? If so, what is the precise sense in which the LQC dynamics reduces to that of WDW theory in such a limit?

The purpose of this (and the accompanying [19]) paper is to address these questions. Two key ideas will make this task feasible. First, we introduce a new representation in both LQC and the WDW theory in which the operator conjugate to volume is diagonal. In this representation, the Hamiltonian constraint of LQC becomes a *differential* operator just as in the WDW theory (for the same reasons as in [16–18]). Second, we will introduce a harmonic time coordinate —which is tailored to the scalar field clock— already at the classical level. This will simplify the factor ordering of the Hamiltonian constraint relative to [3] and make the model exactly soluble. In fact, in the WDW as well as in this soluble LQC theory the Hamiltonian constraint reduces just to the 2-dimensional Klein-Gordon operator! The physical Hilbert space of both theories is then identical (except for a certain global symmetry). How can the theories then lead to strikingly different results on resolution of singularity? The answer of course is that the (Dirac) observables are represented by distinct operators. Thus, in the new representation, one can compare the two theories just by studying the relation between two sets of operators on the *same* Hilbert space. Furthermore, in this representation the expression of Dirac observables is rather simple. Therefore, one can analytically compute the expectation values and dispersions. We find that in the WDW theory the expectation value of the volume operator on a *dense set of states* goes to zero in the distant past (or future). Thus, for a generic state matter density diverges in the distant past (or distant future). In this sense the singularity is unavoidable in the WDW theory. In LQC by contrast, on a dense sub-space the expectation value of the volume operator has a non-zero minimum and diverges both in the distant past and future. Thus, the density remains finite and undergoes a bounce. In this sense the quantum bounce is generic and not tied just to semi-classical states.³ The simplified model also enables us to show that matter density has a finite upper bound $\rho_{\text{sup}} = \sqrt{3}/32\pi^2\gamma^3 G^2 \hbar \approx 0.41\rho_{\text{Pl}}$ on the physical Hilbert space (where γ is the Barbero-Immirzi parameter of LQC). This value coincides exactly with that of the critical density ρ_{crit} [3, 4]! Since the bound is established analytically and without restriction to states which are semi-classical at late times, it provides a deeper understanding of the bounce scenario.

Finally, we analyze the precise sense in which the WDW theory can be regarded as the continuum limit of LQC. We show that given any *fixed, finite* interval I of internal time we can shrink (by hand) the area gap Δ sufficiently so that the WDW theory agrees with LQC to any pre-specified degree of accuracy. However, this approximation is not uniform in I ; the WDW theory cannot approximate LQC for *all* times no matter how much we shrink the area gap. Furthermore, LQC does not admit a limit at all if the gap is shrunk to zero size.

³ The accompanying paper [19] analyzes dispersions of the volume operator in this solvable LQC.

In this sense it is intrinsically discrete, very different from the ‘polymer quantum mechanics’ of a harmonic oscillator [16–18]. We wish to emphasize, however, that all these results refer only to FRW models with a massless scalar field.

We conclude this section with a general observation on singularity resolution. Recall that in classical general relativity, it is non-trivial to obtain necessary and sufficient conditions to characterize the occurrence of a singularity (for example, a space-time can be singular even if all its curvature invariants vanish). It is therefore not surprising that a generally applicable and satisfactory notion of ‘singularity resolution’ is not available in quantum gravity. However, in simple situations such as homogeneous cosmologies the notion of a singularity is unambiguous in the classical theory. In the quantum theory of these models one can also provide a satisfactory notion of singularity resolution. First, one should have available the physical Hilbert space (not just the solutions to constraints) and a complete family of Dirac observables, at least some of which diverge at the singularity. Then one would say that the singularity is resolved if the expectation values of these observables remain finite in the regime in which they become classically singular. In the model studied in this paper, we have a well defined physical inner product as well as a complete set of Dirac observables both in the WDW theory and LQC. In the WDW theory the singularity is not resolved because the expectation value of the matter density diverges at the putative classical singularities while in LQC the singularity is resolved because the expectation values of a complete set of Dirac observables including the matter density remain finite.⁴

The paper is organized as follows. In section II we introduce the new representation in the WDW theory. Section III introduces the simplification in the LQC Hamiltonian constraint and the new representation in which this constraint becomes a differential operator. Section IV compares and contrasts the WDW theory and LQC and section V provides an analytical understanding of two striking features of LQC. In section VI we summarize the results and compares them with analogous discussions in the literature.

II. THE WDW THEORY

It is well known that the WDW theory of the $k=0$ FRW models with a massless scalar field is simple because with an appropriate choice of variables the Hamiltonian constraint can be cast as a 2-dimensional Klein-Gordon equation (see, e.g., [2, 20]). The purpose of this section is to present this theory in a form that makes its relation to LQC easier to analyze. For this, we will need to introduce certain variables and notation which may appear contrived from the internal viewpoint of the WDW theory, but which will facilitate comparison between the two theories in section IV.

⁴ Sometimes apparently weaker notions of singularity resolution are discussed. Consider two examples [13]. One may be able to show that the wave function vanishes at points of the classically singular regions of the configuration space. However, if the *physical* inner product is non-local in this configuration space—as the group averaging procedure often implies—vanishing of the wave function would not imply that the probability of finding the universe at these configurations is zero. The second example is that the wave function may become highly non-classical. This by itself would not mean that the singularity is avoided unless one can show that the expectation values of a family of Dirac observables which become classically singular remain finite there.

To construct a Hamiltonian formulation of the $k=0$ model, one has to introduce a finite fiducial cell \mathcal{V} and restrict all integrations to it [11, 21]. It is easiest to fix a fiducial flat metric \mathring{q}_{cd} and let \mathcal{V} be a cube of volume \mathring{V} with respect to \mathring{q}_{cd} . The standard canonically conjugate variables are $(a, p_{(a)})$ for geometry and $(\phi, p_{(\phi)})$ for the scalar field. Here a is the scale factor relative to \mathring{q}_{cd} : the physical metric q_{cd} being given by $q_{cd} = a^2 \mathring{q}_{cd}$. To compare with LQC, we will make a series of transformations on the geometrical pair $(a, p_{(a)})$.

First, it is convenient to fix a fiducial co-triad $\mathring{\omega}_a^i$ which is orthonormal with respect to \mathring{q}_{cd} and consider co-triads ω_a^i which are orthonormal with respect to q_{cd} so that $\omega_a^i = a \varepsilon \mathring{\omega}_a^i$, where $\varepsilon = 1$ if ω_a^i has the same orientation as the fiducial $\mathring{\omega}_a^i$ and $\varepsilon = -1$ if the orientation is opposite. Second, it is convenient to replace the scale factor a by a variable ν which is proportional to volume (of the cell \mathcal{V}). Let us set

$$\nu = \varepsilon \frac{a^3 \mathring{V}}{2\pi \ell_{\text{Pl}}^2 \gamma} \quad (2.1)$$

where γ is a constant (the Barbero-Immirzi parameter of loop quantum gravity) and $\ell_{\text{Pl}} = (G\hbar)^{1/2}$ is the Planck length. Thus ν has the dimension of length and, because of the orientation factor ε , is not required to be positive; it ranges over $(-\infty, \infty)$. A canonically conjugate variable is given by

$$\mathbf{b} = -\varepsilon \frac{4\pi\gamma G}{3\mathring{V}} \frac{p_{(a)}}{a^2}, \quad (2.2)$$

which has dimensions of inverse length. In quantum theory, the corresponding operators then satisfy the commutation relations:

$$[\hat{\mathbf{b}}, \hat{\nu}] = 2i. \quad (2.3)$$

To construct the Hilbert space of states, we can either use a representation in which $\hat{\nu}$ is diagonal or $\hat{\mathbf{b}}$ is diagonal. In both cases the Hamiltonian constraint becomes a linear, second order differential operator. Thus both representations are simple and neither has a particular advantage over the other. In LQC on the other hand, although the two corresponding representations are again equivalent, in the ν representation physical states turn out to have support on a discrete set of values $\nu = 4n\lambda$, and the geometric part of the Hamiltonian constraint is a *difference* operator on states $\Psi(\nu)$ [3]. Here n is an integer and λ is the square-root of the smallest non-zero eigenvalue $\Delta \ell_{\text{Pl}}^2$ of area. In the \mathbf{b} representation, on the other hand, states $\Psi(\mathbf{b})$ have support on the continuous interval $(0, \pi/\lambda)$ and the geometrical part of the Hamiltonian constraint is represented by a second order *differential* operator.⁵ Consequently comparison between LQC and the WDW theory is most direct in the \mathbf{b} representation. We will therefore let the states be wave functions $\underline{\chi}(\mathbf{b})$ also in the WDW theory. (As in [2, 3], symbols with underbars will refer to the WDW theory.)

In this representation, the Hamiltonian constraint takes the form

$$\partial_\phi^2 \underline{\chi}(\mathbf{b}, \phi) = 12\pi G (\mathbf{b} \partial_{\mathbf{b}})^2 \underline{\chi}(\mathbf{b}, \phi). \quad (2.4)$$

⁵ An analogy with a particle moving on a circle makes this situation transparent. The \mathbf{b} representation in LQC is analogous to the θ -representation in which the states $\Psi(\theta)$ have support on the interval $(0, 2\pi)$ while the ν representation of LQC is analogous to the representation in which p_θ is diagonal so the wave-functions $\Psi(p_\theta)$ have support on discrete values $p_\theta = n\hbar$

In the classical theory, ϕ is monotonic along all dynamical trajectories and therefore serves as an intrinsic clock. As explained in [2], because of the form of the Hamiltonian constraint, this interpretation carries over to quantum theory both in the WDW theory as well as LQC. Physical states must satisfy (2.4). Furthermore, they must satisfy a symmetry requirement. Under change in orientation of the physical co-triad, $(\omega_a^i) \rightarrow \Pi(\omega_a^i) := -\omega_a^i$, the spatial metric does not change and, since there are no fermions in the model, physics remains unchanged. Therefore, this change represents a large gauge transformation. Recall that in Yang-Mills theory physical states belong to *irreducible* representations of the group of large gauge transformations (i.e., to the so-called ‘theta’ sectors). The same reasoning applies to the present case. However, now the large gauge transformation Π satisfies $\Pi^2 = 1$, whence wave functions are either symmetric or anti-symmetric under this action.⁶ Therefore, it suffices to restrict oneself to just the positive (or negative) \mathfrak{b} -half line. For concreteness, let us use the positive half line.

Then, as in the standard WDW theory one can simplify the Hamiltonian constraint by replacing \mathfrak{b} with y which ranges over $(-\infty, \infty)$:

$$y := \frac{1}{\sqrt{12\pi G}} \ln \frac{\mathfrak{b}}{\mathfrak{b}_o} \quad \text{or, equivalently} \quad \mathfrak{b} = \mathfrak{b}_o e^{\sqrt{12\pi G}y} \quad (2.5)$$

where \mathfrak{b}_o is a constant of dimensions of inverse length. The constraint now reduces just to the Klein-Gordon equation in (y, ϕ) :

$$\partial_\phi^2 \underline{\chi}(y, \phi) = \partial_y^2 \underline{\chi}(y, \phi) =: -\underline{\Theta} \underline{\chi}(y, \phi). \quad (2.6)$$

The physical Hilbert space can be obtained by the group averaging procedure used in loop quantum gravity [2, 22–24]. As usual, the procedure tells us that the physical states can be taken to be positive frequency solutions to (2.6), i.e., solutions to

$$-i\partial_\phi \underline{\chi}(y, \phi) = \sqrt{\underline{\Theta}} \underline{\chi}(y, \phi). \quad (2.7)$$

Thus, if the initial data at the intrinsic time $\phi = \phi_o$ is $\underline{\chi}(y, \phi_o) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{-iky} \tilde{\underline{\chi}}(k)$, then the physical state is the solution

$$\begin{aligned} \underline{\chi}(y, \phi) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{-iky + i|k|(\phi - \phi_o)} \tilde{\underline{\chi}}(k) \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^0 dk e^{-ik(\phi+y)} e^{ik\phi_o} \tilde{\underline{\chi}}(k) + \frac{1}{\sqrt{2\pi}} \int_0^{\infty} dk e^{ik(\phi-y)} e^{-ik\phi_o} \tilde{\underline{\chi}}(k) \\ &=: \underline{\chi}_L(y_+) + \underline{\chi}_R(y_-), \end{aligned} \quad (2.8)$$

where $y_\pm = \phi \pm y$ and the subscripts L and R denote left and right moving states. The group averaging procedure also implies that the scalar product is the standard one from Klein-Gordon theory:

$$\begin{aligned} (\underline{\chi}_1, \underline{\chi}_2)_{\text{phy}} &= -i \int_{\phi=\phi_o} dy \left[\bar{\underline{\chi}}_1(y, \phi) \partial_\phi \underline{\chi}_2(y, \phi) - (\partial_\phi \bar{\underline{\chi}}_1(y, \phi)) \underline{\chi}_2(y, \phi) \right] \\ &= 2 \int_{-\infty}^{\infty} dk |k| \bar{\tilde{\underline{\chi}}}_1(k) \tilde{\underline{\chi}}_2(k). \end{aligned} \quad (2.9)$$

⁶ Detailed considerations imply that physical states $\underline{\chi}(\mathfrak{b})$ used here are Fourier transforms of $\underline{\Psi}(\nu)/\nu$ where $\underline{\Psi}(\nu)$ are the states used in [2–4]. Because of the extra $1/\nu$ factor, $\underline{\chi}(\mathfrak{b})$ are anti-symmetric in the WDW theory (as well as in LQC). But this fact will not play an essential role in the subsequent discussion.

We will denote the resulting physical Hilbert space by $\mathcal{H}_{\text{phy}}^{\text{wdw}}$. It is obvious from (2.8) and (2.9) that the left and right moving sectors of $\mathcal{H}_{\text{phy}}^{\text{wdw}}$ are mutually orthogonal. We will see in section IV that physically the left moving component $\underline{\chi}_L$ corresponds to the expanding branch of FRW space-times while and the right moving component $\underline{\chi}_R$, to the contracting branch. (Had we worked with the $\mathbf{b} < 0$ half line the correspondence would have reversed.) It is useful to note that the inner product can also be written as:

$$(\underline{\chi}_1, \underline{\chi}_2)_{\text{phy}} = 2 \int_{-\infty}^{\infty} dy \underline{\chi}_1^{\bar{}}(y, \phi_o) |i\partial_y| \underline{\chi}_2(y, \phi_o) \quad (2.10)$$

where the absolute value denotes the positive part of the self-adjoint operator $i\partial_y$.

Our next task is to define a convenient set of Dirac observables. Since in the classical theory $V|_{\phi_o}$, the volume (of the fiducial cell) at any instant ϕ_o of internal time, is a Dirac observable, in the quantum theory we wish to define a self-adjoint operator $\hat{V}|_{\phi_o}$ on $\mathcal{H}_{\text{phy}}^{\text{wdw}}$. With this goal in mind, let us first introduce the Schrödinger Hilbert space \mathcal{H}_{sch} by freezing physical states at $\phi = \phi_o$ and evaluating the scalar product (2.10) at $\phi = \phi_o$, and define a self-adjoint operator $\hat{\nu}$ on it. Since ν and \mathbf{b} are canonically conjugate, we are led to define

$$\begin{aligned} \hat{\nu} &:= \text{Self-adjoint part of } -2i\partial_{\mathbf{b}} \\ &\equiv \text{Self-adjoint part of } \frac{-2i}{\sqrt{12\pi G \mathbf{b}_o}} e^{-\sqrt{12\pi G} y} \partial_y. \end{aligned} \quad (2.11)$$

Using the fact that the operator $i\partial_y$ is a positive definite self-adjoint operator on the right sector $\mathcal{H}_{\text{sch}}^R$ of \mathcal{H}_{sch} and negative-definite on the left sector $\mathcal{H}_{\text{sch}}^L$, one can easily show that for all smooth functions $\underline{\chi}_1$ and $\underline{\chi}_2$ which fall off sufficiently fast at $y = \pm\infty$, we have

$$\begin{aligned} (\underline{\chi}_1, -2i\partial_{\mathbf{b}} \underline{\chi}_2)_{\text{sch}} &= -\frac{4}{\sqrt{12\pi G \mathbf{b}_o}} \int_{-\infty}^{\infty} dy \left[(\overline{i\partial_y \underline{\chi}_1^R}) e^{-\sqrt{12\pi G} y} (i\partial_y \underline{\chi}_2^R) - (\overline{i\partial_y \underline{\chi}_1^L}) e^{-\sqrt{12\pi G} y} (i\partial_y \underline{\chi}_2^L) \right. \\ &\quad \left. + (\overline{i\partial_y \underline{\chi}_2^R}) e^{-\sqrt{12\pi G} y} (i\partial_y \underline{\chi}_2^L) - (\overline{i\partial_y \underline{\chi}_1^L}) e^{-\sqrt{12\pi G} y} (i\partial_y \underline{\chi}_2^R) \right] \end{aligned} \quad (2.12)$$

where the integral is performed at $\phi = \phi_o$. By calculating the matrix element of the adjoint of $-2i\partial_{\mathbf{b}}$ and adding we obtain the matrix elements of $\hat{\nu}$:

$$(\underline{\chi}_1, \hat{\nu} \underline{\chi}_2)_{\text{sch}} = -\frac{4}{\sqrt{12\pi G \mathbf{b}_o}} \int_{-\infty}^{\infty} dy \left[(\overline{i\partial_y \underline{\chi}_1^R}) e^{-\sqrt{12\pi G} y} (i\partial_y \underline{\chi}_2^R) - (\overline{i\partial_y \underline{\chi}_1^L}) e^{-\sqrt{12\pi G} y} (i\partial_y \underline{\chi}_2^L) \right] \quad (2.13)$$

Therefore, the desired operator $\hat{\nu}$ on \mathcal{H}_{sch} is given by

$$\hat{\nu} = -\frac{2}{\mathbf{b}_o \sqrt{12\pi G}} [P_R(e^{\sqrt{12\pi G} y} i\partial_y) P_R + P_L(e^{\sqrt{12\pi G} y} i\partial_y) P_L] \quad (2.14)$$

where P_R and P_L are projectors on $\mathcal{H}_{\text{sch}}^R$ and $\mathcal{H}_{\text{sch}}^L$. We will now use this expression to define a 1-parameter family of (relational) Dirac observables $\hat{V}|_{\phi_o}$ on $\mathcal{H}_{\text{phy}}^{\text{wdw}}$:

$$\hat{V}|_{\phi_o} \underline{\chi}(y, \phi) = e^{i\sqrt{\bar{\Omega}}(\phi - \phi_o)} (2\pi\gamma \ell_{\text{Pl}}^2 |\hat{\nu}|) \underline{\chi}(y, \phi_o). \quad (2.15)$$

Thus the action of $\hat{V}|_{\phi_o}$ is obtained by first freezing the positive frequency solution $\underline{\chi}(y, \phi)$ at $\phi = \phi_o$, acting on it by the volume operator $2\pi\gamma \ell_{\text{Pl}}^2 |\hat{\nu}|$ and evolving the resulting function

of y using (2.7). (The operator $|\hat{\nu}|$ is the positive part of $\hat{\nu}$ on \mathcal{H}_{sch} .) $\hat{V}|_{\phi_o}$ is a well-defined, self-adjoint operator on $\mathcal{H}_{\text{phy}}^{\text{wdw}}$ because $\hat{\nu}$ enjoys these properties on \mathcal{H}_{sch} .

The second Dirac observable is much simpler: the momentum $\hat{p}_{(\phi)} = -i\hbar\partial_\phi$. Since it is a constant of motion, it is obvious that it preserves the space of solutions to (2.7) and is self-adjoint on $\mathcal{H}_{\text{phy}}^{\text{wdw}}$. Finally, we note that $\hat{V}|_\phi$ and $\hat{p}_{(\phi)}$ preserves each of the left and right moving sectors. Since these constitute a complete set of Dirac observables on $\mathcal{H}_{\text{phy}}^{\text{wdw}}$, there is superselection and one can analyze physics of each of these sectors *separately*.

Let us summarize by focusing on the left moving sector for concreteness. In the more intuitive Schrödinger representation, physical states are functions $\chi_L(y)$ whose Fourier transform $\tilde{\chi}_L(k)$ has support on the negative half of the k -axis and which have finite norm (2.10). The matrix elements of the basic operators are given by

$$\begin{aligned} (\underline{\chi}_L, \hat{p}_{(\phi)} \underline{\chi}'_L)_{\text{phy}} &= 2\hbar \int_{-\infty}^{\infty} dy \partial_y \tilde{\chi}_L(y, \phi_o) \partial_y \underline{\chi}'_L(y, \phi_o) \quad \text{and} \\ (\underline{\chi}_L, |\hat{\nu}|_{\phi_o} \underline{\chi}'_L)_{\text{phy}} &= \frac{4}{\sqrt{12\pi G} \mathbf{b}_o} \int_{-\infty}^{\infty} dy \partial_y \underline{\chi}_L(y, \phi_o) e^{-\sqrt{12\pi G} y} \partial_y \underline{\chi}'_L(y, \phi_o). \end{aligned} \quad (2.16)$$

where ϕ_o is an arbitrary instant of internal time. Note that $\hat{\nu}$ leaves the left sector invariant and is positive definite on it. Hence, $(\underline{\chi}_L, |\hat{\nu}|_{\phi_o} \underline{\chi}'_L)_{\text{phy}} = (\underline{\chi}_L, |\hat{\nu}|_{\phi_o} \underline{\chi}'_L)_{\text{phy}}$. Finally, dynamics is governed by the Schrödinger equation (2.7).

Remark: In the \mathbf{b} representation, the entire theory can be constructed without any reference to the constant \mathbf{b}_o . In the y representation by contrast the constant \mathbf{b}_o appears even in the final theory through the expression of the operator $\hat{\nu}$. (As we just saw, the inner product and the expression of the other Dirac observable $\hat{p}_{(\phi)}$ is independent of \mathbf{b}_o also in the y -representation.) However, it is easy to verify that change in \mathbf{b}_o just yields a unitarily equivalent theory (as it must). To make this explicit, denote by y' the left side of (2.5) obtained by replacing \mathbf{b}_o with \mathbf{b}'_o . Let us again restrict ourselves to the left moving sector. Then the theory based on \mathbf{b}_o is mapped to that based on $\mathbf{b}'_o = \alpha\mathbf{b}_o$ by the operator \hat{U}_α : $\hat{U}_\alpha\chi(y) = \chi'(y') := \chi(y' + \ln \alpha / \sqrt{12\pi G})$. This is a unitary map which preserves $\hat{p}_{(\phi)}$ and sends $\hat{\nu}$ to $\hat{\nu}'$, i.e., has the action

$$\hat{U} \left[\frac{2i}{\sqrt{12\pi G} \mathbf{b}_o} \exp(-\sqrt{12\pi G} y) \partial_y \right] \hat{U}^{-1} = \frac{2i}{\sqrt{12\pi G} \mathbf{b}'_o} \exp(-\sqrt{12\pi G} y') \partial_{y'}. \quad (2.17)$$

III. SOLVABLE LQC

This section is divided into three parts. In the first, for convenience of the reader we present a brief summary of LQC including a short explanation of the necessity of ‘improved’ dynamics of [3, 4]. These references began with the Hamiltonian constraint corresponding to proper time in the classical theory and changed to the internal time defined by the scalar field only after quantization. In the second sub-section we follow an alternate strategy: we use a ‘harmonic time coordinate’ (tailored to the use of the scalar field as an internal clock) already in the classical theory. Then the quantum Hamiltonian constraint acquires a slightly different factor ordering. But this difference turns out to suffice to enable one to solve the quantum theory exactly. (The precise relation between the two strategies is discussed in the Appendix A.) In the third subsection we introduce the \mathbf{b} representation in which the LQC Hamiltonian constraint becomes a differential operator, facilitating comparison with the WDW theory in section IV.

A. Dynamics of LQC

As in the WDW theory, because of spatial homogeneity and non-compactness of the spatial manifold, to construct the Hamiltonian formulation one has to introduce an elementary cell \mathcal{V} and restrict all integrations to it. (This is necessary also in the path integral treatment based on Lagrangians.) Let us then introduce fiducial co-triads $\mathring{\omega}_a^i$ and triads \mathring{e}_i^a which define a flat metric \mathring{q}_{ab} and choose \mathcal{V} to be a cubical cell whose sides are aligned with the three e_i^a . Symmetries imply that, by a suitable gauge fixing, the basic canonical pair (A_a^i, E_i^a) of loop quantum gravity (LQG) can be chosen to have the form [11]

$$A_a^i = c \mathring{V}^{-1/3} \mathring{\omega}_a^i, \quad \text{and} \quad E_i^a = p \sqrt{\det \mathring{q}} \mathring{V}^{-2/3} \mathring{e}_i^a \quad (3.1)$$

where, as before, \mathring{V} is the volume of \mathcal{V} with respect to the fiducial metric \mathring{q}_{ab} . The dynamical variables are thus just c and p . The factors of \mathring{V} are chosen so that the Poisson brackets between them are independent of \mathring{V} :

$$\{c, p\} = \frac{8\pi\gamma G}{3}. \quad (3.2)$$

Note that p ranges over the whole real line, being positive when the physical triad e_i^a has the same orientation as the fiducial \mathring{e}_i^a and negative when the orientations are opposite. c is dimensionless while p has dimensions of area. The two are related to the scale factor via $p = \varepsilon a^2$ (where as before $\varepsilon = \pm 1$ is the orientation factor), and $c = \gamma \dot{a}$ (on classical solutions).

In the LQC Hilbert space, the eigenbasis $|p\rangle$ of \hat{p} is adapted to quantum geometry. The *physical* volume of the elementary cell \mathcal{V} is simply $|p|^{3/2}$, i.e. $\hat{V}|p\rangle = |p|^{3/2}|p\rangle$. The geometrical part of the Hamiltonian constraint in the connection variables involves the (density weighted) physical triads E_i^a and the field strength F_{ab}^i of the gravitational connection A_a^i . The factors involving E_i^a can be quantized [11] using techniques introduced by Thiemann [25, 26] in full LQG. The field strength F_{ab}^i is more subtle because a fundamental feature of LQG is that while holonomy operators are well-defined, there is no operator directly corresponding to the connection [27, 28]. Therefore, as in gauge theories, components of F_{ab}^i have to be recovered by considering holonomies around suitable loops, dividing them by the area they enclose, and then shrinking these loops.

In the earlier LQC treatments [11], this area was calculated using the *fiducial* metric. The geometrical part of the Hamiltonian constraint was then a difference operator with uniform steps in p , the step size being dictated by the minimum non-zero area eigenvalue $2\sqrt{3}\pi\gamma\ell_{\text{Pl}}^2 \equiv \Delta\ell_{\text{Pl}}^2$. The resulting dynamics resolves the singularity, replacing the big bang by a big bounce. However, detailed investigation [2] showed that this dynamics has several unphysical features. First, for semi-classical states, the density at which the bounce occurs depends on the expectation value $\hat{p}_{(\phi)}$ in the state, $\rho_{\text{bounce}} = (1/18\pi G\gamma^2)^{3/2} (1/\sqrt{2}|p_{(\phi)}|)$. Now, $\hat{p}_{(\phi)}$ is a constant of motion and the higher the value of $p_{(\phi)}$ the more semi-classical the state is. (For example, in the closed, $k=1$ model the value of p_ϕ determines the maximum volume of the universe V_{max} . The larger the value of p_ϕ , the larger is V_{max}). Thus, more semi-classical the state, lower is the density at which the bounce occurs, whence the theory predicts that there can be gross departures from classical general relativity even at density of water! Second, such departures are not confined just to the bounce. In presence of a cosmological constant Λ they occur also in a ‘tame’ region well away from the classical singularity, where $a^2 \Lambda \equiv |p| \Lambda \gtrsim 1$. Finally, even qualitative features of the final quantum

dynamics can depend on the choice of the initial fiducial cell \mathcal{V} (see Appendix B.2 in [3]). The cell is just an auxiliary structure needed in the mathematical framework. Therefore, while it is acceptable that intermediate steps in the calculation depend on this ‘gauge choice’, the final physical predictions must not.

The ‘improved dynamics’ of [3, 4] is based on the realization that all these limitations stem from the fact that *fiducial* geometry was used in quantization of F_{ab}^i . If area in this calculation refers instead to the *physical* geometry, the subsequent mathematics realigns itself just in the right way to cure all these problems. The density ρ_{crit} at the bounce is now a constant, $\rho_{\text{crit}} = \sqrt{3}/(32\pi^2\gamma^3 G^2 \hbar) \approx 0.41\rho_{\text{Pl}}$, which is independent of $p(\phi)$ and therefore has no implicit dependence on the choice of the fiducial cell \mathcal{V} . In presence of a cosmological constant, departures from general relativity occur only if the curvature enters the Planck regime; general relativity continues to be an excellent approximation away from the singularity, improving steadily as the scale factor a increases. Thus, the limitations of the older dynamics stem from the fact that it uses a mathematically variable but physically incorrect notion of area in defining the operator analog of F_{ab}^i . Indeed quanta of area —i.e. eigenvalues of the area operator— should refer to the physical geometry not to a kinematical background.

B. The Hamiltonian constraint

It turns out that the geometrical part of the ‘improved’ Hamiltonian constraint [3] is a difference operator with uniform step size, but now in volume ($\sim a^3$) rather than p ($\sim a^2$). Therefore, it is convenient to use a representation in which states are wave functions $\tilde{\Psi}(\nu)$, where ν is given by (2.1), so that the operator \hat{V} measuring the volume of the elementary cell \mathcal{V} is given by⁷

$$\hat{V}\tilde{\Psi}(\nu) = 2\pi\ell_{\text{Pl}}^2\gamma|\nu|\tilde{\Psi}(\nu). \quad (3.3)$$

As before, the variable \mathbf{b} of (2.2) is canonically conjugate to ν . However, whereas $\hat{\nu}$ is a well-defined operator, $\hat{\mathbf{b}}$ is no longer well-defined in LQC because now there is no operator corresponding to the connection. Nevertheless, since the holonomies are well-defined, $\widehat{\exp i\lambda\mathbf{b}}$ is a well-defined operator, with action

$$\widehat{\exp i\lambda\mathbf{b}}\tilde{\Psi}(\nu) = \tilde{\Psi}(\nu + 2\lambda) \quad (3.4)$$

where λ is an arbitrary parameter with dimensions of length.

Since we wish to use the scalar field ϕ as an internal time variable and since ϕ satisfies the wave equation $\square\phi = 0$, it is natural to use a harmonic gauge in which the time variable τ satisfies $\square\tau = 0$. The corresponding space-time metric takes the form:

$$ds^2 = a^6 d\tau^2 + a^2 d\vec{x}^2 \quad (3.5)$$

where $a \equiv a(\tau)$ is the scale factor. (It is easy to verify that τ automatically satisfies $\square\tau = 0$ with respect to this metric.) Because the lapse function is now given by $N = a^3$, the

⁷ In [2–4], states were chosen to be functions of a dimensionless parameter v in terms of which volume eigenvalues are $(8\pi\gamma/6)^{3/2}(|v|/K)\ell_{\text{Pl}}^3$ where $K = 2\sqrt{2}/3\sqrt{3\sqrt{3}}$. Thus, v is related to the present ν by $v = 2/\sqrt{8\pi\gamma\sqrt{3}}(\nu/\ell_{\text{Pl}})$. This is a trivial change of variables to simplify the expression of the Hamiltonian constraint.

Hamiltonian constraint becomes

$$p_{(\phi)}^2 - \frac{3}{4\pi G\gamma^2} p^2 c^2 = 0. \quad (3.6)$$

The key simplification is the absence of inverse powers of the scale factor.⁸ This simplification is sufficient to make the model analytically solvable. *Therefore, we will call the resulting model solvable LQC and denote it by sLQC.* This labeling will serve to distinguish the factor ordering used here from that used in [3, 4].

The “improved dynamics” procedure used in [3] now leads to the quantum constraint:

$$\partial_\phi^2 \tilde{\Psi}(\nu, \phi) = 3\pi G |\nu| \frac{\sin \lambda \mathbf{b}}{\lambda} |\nu| \frac{\sin \lambda \mathbf{b}}{\lambda} \tilde{\Psi}(\nu, \phi) \quad (3.7)$$

where λ is now the (positive) square-root of the area gap: $\lambda^2 = \Delta \ell_{\text{Pl}}^2 \equiv 2\sqrt{3} \pi \gamma \ell_{\text{Pl}}^2$. Since one of the goals of this paper is to spell out the relation between LQC and the WDW theory, we want to retain the ability of sending the area gap to zero. Therefore *we will leave λ as a free parameter, $\lambda \leq \sqrt{\Delta} \ell_{\text{Pl}}$, rather than fixing it to the LQC value $\lambda = \sqrt{\Delta} \ell_{\text{Pl}}$.*

Next, as in the WDW theory, physical states have to satisfy a symmetry requirement. Under orientation reversal Π of physical triads e_i^a , $\nu \rightarrow \Pi(\nu) = -\nu$. This is a large gauge transformation. As discussed in section II, following the standard procedure from gauge theories, physical states belong to irreducible representations of the group of large gauge transformations. Since there are no fermions in this model, in LQC $\tilde{\Psi}$ is assumed to be symmetric: $\Pi \tilde{\Psi}(\nu, \phi) := \tilde{\Psi}(-\nu, \phi) = \tilde{\Psi}(\nu, \phi)$.

Using this symmetry and writing out the explicit action of operators $\sin \lambda \mathbf{b}$, (3.7) simplifies to:

$$\begin{aligned} \partial_\phi^2 \tilde{\Psi}(\nu, \phi) &= 3\pi G \nu \frac{\sin \lambda \mathbf{b}}{\lambda} \nu \frac{\sin \lambda \mathbf{b}}{\lambda} \tilde{\Psi}(\nu, \phi) \\ &= \frac{3\pi G}{4\lambda^2} \nu \left[(\nu + 2\lambda) \tilde{\Psi}(\nu + 4\lambda) - 2\nu \tilde{\Psi}(\nu) + (\nu - 2\lambda) \tilde{\Psi}(\nu - 4\lambda) \right] \\ &=: \Theta_{(\nu)} \tilde{\Psi}(\nu, \phi). \end{aligned} \quad (3.8)$$

The geometrical part, $\Theta_{(\nu)}$, of the constraint is a difference operator in steps of 4λ . Hence, as discussed in [3, 4], there is again superselection: for each $\epsilon \in [0, 4\lambda)$, the space of states $\tilde{\Psi}(\nu)$ with support on points $\nu = \epsilon + 4n\lambda$ is preserved under dynamics. In this paper we will focus on the $\epsilon = 0$ ‘lattice’ which is invariant under Π .

C. Reducing the sLQC constraint to a Klein-Gordon Equation

For reasons explained in the Introduction, we now wish to work in the \mathbf{b} representation because the geometrical part of the quantum constraint will also become a differential operator. Since $\tilde{\Psi}(\nu, \phi)$ have support on the ‘lattice’ $\nu = 4n\lambda$, and since \mathbf{b} is canonically conjugate

⁸ This strategy was not used in [3, 4] because this choice, $N = a^3$ does not have a natural analog outside homogeneous cosmologies while the choice $N = 1$ used there (which corresponds to using of proper time) is generally available.

to ν , their Fourier transforms $\Psi(\mathbf{b}, \phi)$ have support on the continuous interval $(0, \pi/\lambda)$:

$$\Psi(\mathbf{b}, \phi) := \sum_{\nu=4n\lambda} e^{\frac{i}{2}\nu\mathbf{b}} \tilde{\Psi}(\nu, \phi); \quad \text{so that} \quad \tilde{\Psi}(\nu, \phi) = \frac{\lambda}{\pi} \int_0^{\pi/\lambda} d\mathbf{b} e^{-\frac{i}{2}\nu\mathbf{b}} \Psi(\mathbf{b}, \phi). \quad (3.9)$$

From the form (3.7) of the constraint it is obvious that it would be a second order differential operator in the \mathbf{b} -representation. To facilitate comparison with the WDW theory, let us set $\tilde{\chi}(\nu, \phi) = (\lambda/\pi\nu)\tilde{\Psi}(\nu, \phi)$. Then, on $\chi(\mathbf{b}, \phi)$, the constraint (3.7) becomes

$$\partial_\phi^2 \chi(\mathbf{b}, \phi) = 12\pi G \left(\frac{\sin \lambda\mathbf{b}}{\lambda} \partial_{\mathbf{b}} \right)^2 \chi(\mathbf{b}, \phi) \quad (3.10)$$

which is strikingly similar to the WDW equation (2.4). Note however, that *we did not* arrive at (3.10) simply by replacing \mathbf{b} in the expression of the classical constraint by $\sin \lambda\mathbf{b}/\lambda$ as is often done (see, e.g., [15, 30]). Rather, (3.10) results directly from the ‘improved’ LQC constraint if one begins with a harmonic time coordinate already in the classical theory.

To simplify the constraint further, let us set

$$x = \frac{1}{\sqrt{12\pi G}} \ln\left(\tan \frac{\lambda\mathbf{b}}{2}\right), \quad \text{or} \quad \mathbf{b} = \frac{2}{\lambda} \tan^{-1}\left(e^{\sqrt{12\pi G}x}\right) \quad (3.11)$$

so x ranges from $-\infty$ to ∞ . Then (3.8) becomes just the Klein-Gordon equation

$$\partial_\phi^2 \chi(x, \phi) = \partial_x^2 \chi(x, \phi) =: -\Theta \chi(x, \phi). \quad (3.12)$$

Therefore we can repeat the discussion of section II. The physical Hilbert space is again given by positive frequency solutions to (3.12), i.e. satisfy

$$-i\partial_\phi \chi(x, \phi) = \sqrt{\Theta} \chi(x, \phi). \quad (3.13)$$

We can again express the solutions in terms of their initial data and decompose them into left and right moving modes $\chi(x, \phi) = \chi_L(x_+) + \chi_R(x_-)$ (see Eq (2.8)). The physical inner product is given by (2.9) or, equivalently, (2.10). Thus, the physical Hilbert space of LQC is exactly the same as in the WDW theory and indeed the action of the operator $\hat{p}_{(\phi)}$ on physical states is the same: $\hat{p}_{(\phi)}\chi = -i\hbar\partial_\phi\chi \equiv \sqrt{-\partial_x^2}\chi$.

How can there be difference in physical predictions, then? Recall that to obtain physical predictions, we need the action of a complete set of physical observables and, as we will now show, the volume observable $\hat{V}|_{\phi_o}$ in LQC has a *different* form from that in the WDW theory. Consequently, although the Hilbert spaces are mathematically the same, the *physical meaning* of a given positive frequency solution is different in the two theories.

Let us begin with the operator $\hat{\nu}$ on the Schrödinger Hilbert space \mathcal{H}_{sch} spanned by the initial data $\chi(x, \phi_o)$ to (3.13), where the inner product is obtained by evaluating (2.10) at $\phi = \phi_o$. As in the WDW theory, $\hat{\nu}$ is again the self-adjoint part of $-2i\partial_b$. *However, while $-2i\partial_b = (-2i/\sqrt{12\pi G b_o}) \exp(-\sqrt{12\pi G}y) \partial_y$ in the WDW theory, it is now given by $(-2i\lambda/\sqrt{12\pi G}) \cosh(\sqrt{12\pi G}x) \partial_x$.* Therefore, repeating the procedure we followed in section II, on \mathcal{H}_{sch} the operator $\hat{\nu}$ is given by:

$$\hat{\nu} = -\frac{2\lambda}{\sqrt{12\pi G}} [P_R(\cosh(\sqrt{12\pi G}x) i\partial_x) P_R + P_L(\cosh(\sqrt{12\pi G}x) i\partial_x) P_L]. \quad (3.14)$$

Therefore, as in the WDW theory, the corresponding volume operator on \mathcal{H}_{phy} is given by

$$\hat{V}|_{\phi_o} \chi(x, \phi) = e^{i\sqrt{\Theta}(\phi-\phi_o)} (2\pi\gamma\ell_{\text{Pl}}^2 |\hat{\nu}|) \chi(x, \phi_o). \quad (3.15)$$

A second difference from the WDW theory arises because of symmetry conditions on the physical states. Recall that to qualify as a physical state $\Psi(\nu, \phi)$ has not only to be a positive frequency solution but must also satisfy $\tilde{\Psi}(-\nu, \phi) = \tilde{\Psi}(\nu, \phi)$. This translates to the condition $\chi(-x, \phi) = -\chi(x, \phi)$. Therefore $\chi(x, \phi)$ has the form

$$\chi(x, \phi) = \frac{1}{\sqrt{2}} (F(x_+) - F(x_-)) \quad (3.16)$$

for some function F (such that $F(x_{\pm})$ are positive frequency solutions to (3.12)). Consequently, in contrast to the WDW theory, the right and left sectors are *not* superselected. However, since the full information in any physical state $\chi(x, \phi)$ is contained in F , we can conveniently describe the \mathcal{H}_{phy} in terms of positive frequency, left moving solutions $F(x_+)$ (or, right moving solutions $F(x_-)$) alone, which are free from any symmetry requirement. In this description, the scalar product is given simply by

$$(\chi_1, \chi_2)_{\text{phy}} = -2i \int_{-\infty}^{\infty} dx \bar{F}_1(x_+) \partial_x F_2(x_+) \quad (3.17)$$

where the integral is evaluated at a constant value of ϕ .

Let us summarize the basic structure using a Schrödinger representation which will be useful in the next section. For any given λ , the LQC Hilbert space can be taken to be the space of functions $F(x)$ whose Fourier transform $\tilde{F}(k)$ has support only on the positive half line and whose norm given by (3.17) is finite. Matrix elements of the basic observables $\hat{p}_{(\phi)}$ and $\hat{\nu}$ are given by:

$$\begin{aligned} (F_1, \hat{p}_{(\phi)} F_2)_{\text{phy}} &= 2\hbar \int_{-\infty}^{\infty} dx \partial_x \bar{F}_1(x_+) \partial_x F_2(x_+) \quad \text{and} \\ (F_1, \hat{\nu}|_{\phi_o} F_2)_{\text{phy}} &= \frac{4\lambda}{\sqrt{12\pi G}} \int_{-\infty}^{\infty} dx \partial_x \bar{F}_1(x_+) \cosh(\sqrt{12\pi G}x) \partial_x F_2(x_+) \end{aligned} \quad (3.18)$$

where the integral is evaluated at $\phi = \phi_o$. The states evolve via the Schrödinger equation

$$-i\partial_{\phi} F(x_+) = \sqrt{\Theta} F(x_+) \quad (3.19)$$

so that, as in the WDW theory the effective Hamiltonian is non-local in x . Thus, the only difference from the WDW theory lies in the expression of $\hat{\nu}$ and hence of the volume operator.

Remark: A quick way to arrive at the constraint (3.10) in the \mathbf{b} -representation is to write the classical constraint in terms of the canonical pair (\mathbf{b}, ν) and then simply replace \mathbf{b} by $(\sin \lambda \mathbf{b})/\lambda$ and ν by $-2i\partial_{\mathbf{b}}$. While this so-called ‘polymerization method’ [18, 30] yields the correct final result, it is not directly related to procedures used in LQG. Since ν is a geometrical variable, its quantization could be carried out using quantum geometry techniques. However, \mathbf{b} has no natural analog in LQG. In particular, since it is not a connection component, a priori it is not clear why the wave functions have to be even almost periodic in \mathbf{b} nor why λ should be related to the area gap. For a plausible relation to LQG one has to start with the canonical pair (A_a^i, E_i^a) , i.e., (c, p) , mimic the procedure used in LQG as much as possible, e.g., along the lines of [3], and then pass to the \mathbf{b} representation as was done here. Once this is done, *a posteriori* it is possible, and indeed often very useful, to use shortcuts such as $\mathbf{b} \rightarrow (\sin \lambda \mathbf{b})/\lambda$.

IV. THE WDW THEORY AND LQC: SIMILARITIES AND DIFFERENCES

This section is divided into two parts. In the first we show that there is a precise sense in which the singularity is generic in the WDW theory while it is generically replaced by a quantum bounce in sLQC. In the second we spell out a precise sense in which the WDW theory approximates sLQC and the sense in which this approximation fails.

A. Singularity versus the quantum bounce

In spatially homogeneous, isotropic space-times the only curvature invariant is the space-time scalar curvature which is proportional to the matter density. Classical singularity is characterized by the divergence of these quantities. Now, the matter density is given by $\rho = p_{(\phi)}^2/2V^2$ and since there is no potential for the scalar field, $p_{(\phi)}$ is a constant of motion in our model (also in the quantum theory). Therefore, to answer the question of whether a given quantum state is singular or not, one can calculate the expectation values of the Dirac observable \hat{V}_ϕ . If $\langle \hat{V}_\phi | \phi \rangle$ goes to zero (possibly in the limit as ϕ tends to $\pm\infty$ as in classical general relativity), one can say that the quantum state leads to a singularity. If $\langle \hat{V}_\phi | \phi \rangle$ diverges in both directions, i.e., as $\phi \rightarrow \pm\infty$, but attains a non-zero minimum, one can say that the state exhibits a quantum-bounce. While this is a rather weak criterion, it is applicable to any state (in the domain of the volume operator). In this sense, it enables us to test the generic behavior in the WDW theory and in sLQC, thereby going beyond the analysis of [1–3] which was restricted to states which are semi-classical at late times.

Let us begin with the WDW theory. As noted in section II the left and right moving sector are superselected and can be analyzed separately. For definiteness we will focus on the left moving sector. Then, for any $\underline{\chi}(y_+)$ we have

$$\begin{aligned}
 (\underline{\chi}_L, \hat{V}_\phi | \phi \underline{\chi}_L)_{\text{phy}} &= 2\pi\gamma\ell_{\text{Pl}}^2 (\underline{\chi}_L, |\hat{v}|_{\phi_o} \underline{\chi}_L)_{\text{phy}} \\
 &= \frac{8\pi\gamma\ell_{\text{Pl}}^2}{\sqrt{12\pi G} \mathbf{b}_o} \int_{-\infty}^{\infty} dy \left| \frac{\partial \underline{\chi}_L}{\partial y} \right|^2 e^{-\sqrt{12\pi G}y} \\
 &= \left[\frac{8\pi\gamma\ell_{\text{Pl}}^2}{\sqrt{12\pi G} \mathbf{b}_o} \int_{-\infty}^{\infty} dy_+ \left| \frac{d\underline{\chi}_L}{dy_+} \right|^2 e^{-\sqrt{12\pi G}(y_+)} \right] e^{\sqrt{12\pi G}\phi} \\
 &=: V_o e^{\sqrt{12\pi G}\phi}, \tag{4.1}
 \end{aligned}$$

where V_o is a constant determined by the solution and can be calculated from initial data at any instant of time. Thus, for any state $\underline{\chi}_L(y_+)$ in the domain of the volume operator, the expectation value $\langle \hat{V}_\phi | \phi \rangle$ tends to ∞ as the internal time ϕ tends to ∞ and goes to zero as ϕ tends to $-\infty$. In this sense the left moving sector corresponds to the expanding universes. It is obvious from the above calculation that on the right moving sector $\underline{\chi}_R(y_-)$ the situation would be reversed whence it represents contracting universes. In the first case there is a big bang singularity and in the second, a big crunch singularity. Indeed, states which are semi-classical in an epoch when the density is very low compared to the Planck density are known to follow the classical trajectories into either the big bang or the big-crunch singularity [3]. We have shown that this qualitative behavior is generic: for a dense subset of states, expectation values $\langle \hat{V}_\phi | \phi \rangle$ of the volume operator evolve into a big bang or a big crunch singularity. This calculation also shows that the matter density, defined as

$\tilde{\rho} := \langle \hat{p}(\phi) \rangle^2 / 2 \langle \hat{V} \rangle^2$ diverges as $\phi \rightarrow -\infty$ (resp. $\phi \rightarrow \infty$) in the left (resp. right) moving sector. Furthermore, the same considerations apply to the expectation values of the density operator $\hat{\rho}|_\phi$ because, as shown in section V A, its expectation value has the same behavior as $\tilde{\rho}$.

Let us carry out the same calculation in sLQC. Consider any state $\chi(x, \phi) = (1/\sqrt{2})(F(x_+) - F(x_-))$. Then, we have:

$$\begin{aligned} (\chi, \hat{V}|_\phi \chi)_{\text{phy}} &= 2\pi\gamma\ell_{\text{Pl}}^2 (\chi, |\hat{\nu}|_{\phi_0} \chi)_{\text{phy}} \\ &= \frac{8\pi\gamma\ell_{\text{Pl}}^2\lambda}{\sqrt{12\pi G}} \int_{-\infty}^{\infty} dx \left[\partial_x \bar{\chi}_L \cosh(\sqrt{12\pi G} x) \partial_x \chi_L + \partial_x \bar{\chi}_R \cosh(\sqrt{12\pi G} x) \partial_x \chi_R \right] \\ &= \frac{8\pi\gamma\ell_{\text{Pl}}^2\lambda}{\sqrt{12\pi G}} \int_{-\infty}^{\infty} dx_+ \left| \frac{dF}{dx_+} \right|^2 \cosh(\sqrt{12\pi G}(x_+ - \phi)), \end{aligned}$$

which can be written as

$$(\chi, \hat{V}|_\phi \chi)_{\text{phy}} = V_+ e^{\sqrt{12\pi G}\phi} + V_- e^{-\sqrt{12\pi G}\phi} \quad (4.2)$$

where

$$V_{\pm} = \frac{4\pi\gamma\ell_{\text{Pl}}^2\lambda}{\sqrt{12\pi G}} \left[\int_{-\infty}^{\infty} dx_+ \left| \frac{dF}{dx_+} \right|^2 e^{\mp\sqrt{12\pi G}x_+} \right] \quad (4.3)$$

are again constants associated with the solution which can be calculated from the initial data at any fixed ϕ . Note that V_{\pm} are strictly positive (compare [15]). In contrast to the WDW theory, $\langle \hat{V}|_\phi \rangle$ tends to infinity both in the distant future and in the distant past. Furthermore, it has a *unique* local minimum which is therefore also a global minimum. In this sense the bounce picture of [3, 4] is robust. It is not restricted to states which are semi-classical at late times but holds for all states in the domain of the volume operator. Similarly, since the result is obtained analytically, an apparent concern (which arose from some observations made in [31]) that the presence of the bounce may be related to intricacies of numerics is ill founded. The bounce point and the minimum volume are given by:

$$\phi_{\text{B}} = \frac{1}{2\sqrt{12\pi G}} \log \frac{V_-}{V_+}, \quad \text{and} \quad V_{\text{min}} = 2 \frac{(V_+ V_-)^{\frac{1}{2}}}{\|\chi\|^2}, \quad (4.4)$$

where $\|\chi\|$ is the norm of the state χ .

Next, we note that

$$\langle \hat{V}|_\phi \rangle_{\phi_{\text{B}}+\phi} = V_{\text{min}} \cosh(\sqrt{12\pi G}\phi). \quad (4.5)$$

Therefore, the internal-time evolution of volume is exactly symmetric about the bounce point for *all* states. For reasons just discussed one would expect that the symmetry would hold also in LQC to an excellent degree of approximation. This symmetry was already observed in [3] through numerical and effective equation methods and in [15] using a simplified model. However, all these analyses were tied to various notions of semi-classicality. Our results overcome the concern that the symmetry may not extend to general states. Our considerations here refer only to expectation values. However, the same techniques are used in [19] to calculate fluctuations of the volume operator and analyze its properties.

Remark: In the WDW theory the left and right sectors are superselected and should therefore be considered separately. Nonetheless, since in sLQC all physical states χ satisfy $\sqrt{2}\chi(x, \phi) = F(x_+) - F(x_-)$ for some F , one may be tempted to consider states $\underline{\chi}(y, \phi)$ which

are similarly anti-symmetric in y also in the WDW theory. This strategy would however be physically incorrect because of two reasons. First, the anti-symmetry condition in x arises in sLQC because physics is symmetric under reflections of spatial triads E_i^a . This condition has already been incorporated in the WDW theory in arriving at the y representation. Secondly, if one were nonetheless to impose anti-symmetry in the WDW theory, one would find that this sector does not have any semi-classical states at very late (or very early) times because, in this sector, states which are peaked at large volume would have very large —rather than small— extrinsic curvature.

B. Approximating sLQC with the WDW theory

There is a precise sense in which the WDW equation approximates the LQC evolution equation [2, 3, 11]. However, as is well known, the issue of whether solutions to two such equations approximate each other is logically quite distinct. In particular the equations may be such that initial data satisfying the assumptions needed to show that the two equations approximate each other may evolve out of this regime. If this occurs, solutions of the two theories may be close to each other initially but could eventually differ drastically. In this section we will show that this is precisely what happens in our case.

At first this may seem perplexing because in sections II and III we showed that the physical states in both theories satisfy the (positive frequency) Klein-Gordon equation. Isn't then the evolution identical? However, as pointed out in section III C that in quantum theory the physical content of a state lies not in its functional form but in its interplay with observables. While the action of $\hat{p}_{(\phi)}$ is the same in the two theories, the action of $\hat{V}|_\phi$ is distinct (compare (2.16) and (3.18)). Therefore the theories are inequivalent. The question for us is: Can one arrive at the WDW theory by shrinking the area gap of sLQC, i.e., by letting λ go to zero? Again, one cannot naively set λ to zero: λ appears linearly in the expression of the volume operator (see (3.18)) and setting it to zero will make the operator itself zero. Rather, we have to work with states and operators together.

Let us consider the 1-parameter family of Dirac observables $\hat{V}|_\phi$. A *necessary* condition for the WDW theory to approximate sLQC is that, for any state of the WDW theory, there should exist a state of sLQC $_{(\lambda)}$ such that the expectation values of volume operators in the two states can be made arbitrarily close to one another by choosing a sufficiently small λ .⁹ More precisely, given $\epsilon > 0$, there should exist a $\delta > 0$ such that for any state $\underline{\chi}_L(y, \phi)$ of the WDW theory, there is a state $\chi_{(\lambda)}(x, \phi)$ of sLQC $_{(\lambda)}$ such that

$$|\langle \hat{V}|_\phi \rangle_{(\lambda)} - \langle \hat{V}|_\phi \rangle_{\text{wdw}}| < \epsilon \quad (4.6)$$

for all $\lambda < \delta$. Now, the forms (4.1) and (4.2) of the two expectation values

$$\langle \hat{V}|_\phi \rangle_{\text{wdw}} = V_o e^{\sqrt{12\pi G}\phi}, \quad \text{and} \quad \langle \hat{V}|_\phi \rangle_{(\lambda)} = V_+ e^{\sqrt{12\pi G}\phi} + V_- e^{-\sqrt{12\pi G}\phi} \quad (4.7)$$

immediately implies that if (4.6) is to hold for all positive ϕ then

$$V_o = V_+ \quad \text{and} \quad V_- < \epsilon \quad (4.8)$$

⁹ In the $k=0$, spatially non-compact context considered here, one must introduce a finite cell to speak of volume. However, ratios of the volume expectation values $\langle \hat{V}|_\phi \rangle$ at two different times or, at the same time but computed using sLQC and the WDW theory are independent of the choice of the cell.

where V_o is defined by (4.1) using $\underline{\chi}_L(y, \phi)$ and V_{\pm} by (4.3) using $\chi_{(\lambda)}(x, \phi)$. However, since V_- is necessarily positive, it follows that $|\langle \hat{V} |_{\phi} \rangle_{(\lambda)} - \langle \hat{V} |_{\phi} \rangle_{\text{wdw}}|$ will grow unboundedly as $\phi \rightarrow -\infty$ no matter how small δ is. Thus, the necessary condition for the WDW theory to approximate sLQC is violated: the global dynamics of the two theories is very different.

While the simple argument above establishes the main result of this section, it is instructive to examine some details by explicitly constructing a map from $\underline{\chi}_L(y, \phi)$ to $\chi_{(\lambda)}(x, \phi) = (1/\sqrt{2})(F_{(\lambda)}(x_+) - F_{(\lambda)}(x_-))$. For this it is convenient to work in the Schrödinger representation at time, say, $\phi = 0$. Then our task is to construct $F_{(\lambda)}(x)$ from the initial data $\underline{\chi}_L(y, 0)$. Fix an $\epsilon > 0$ and consider the family of Schrödinger states $\underline{\chi}_L(y)$ of the WDW theory for which V_- of (4.3) (obtained by using $\underline{\chi}_L$ for F) satisfies $V_- < \epsilon$. Then, considerations in the remark at the end of section II suggest that we set

$$F_{(\lambda)}(x) := \underline{\chi}_L(x + \mu) \quad \text{where} \quad \mu = \frac{1}{\sqrt{12\pi G}} \ln \frac{2}{b_o \lambda}. \quad (4.9)$$

Then for any λ , the pairs $\underline{\chi}(y)$ and $F_{(\lambda)}(x)$ are Schrödinger states which are ‘close’ to one another at $\phi = 0$ in the sense that:

- i) They have the same norm: $\|\underline{\chi}(y)\|_{\text{phys}}^{\text{wdw}} = \|F_{(\lambda)}(x)\|_{\text{phys}}$; and,
- ii) They have the same expectation values for any power of \hat{p}_{ϕ} : $\langle \hat{p}_{(\phi)}^n \rangle_{\text{wdw}} = \langle \hat{p}_{(\phi)}^n \rangle_{(\lambda)}$; and,
- iii) Their volume expectation values are close: $|\langle \hat{V} |_{\phi} \rangle_{\text{wdw}} - \langle \hat{V} |_{\phi} \rangle_{(\lambda)}| < \epsilon$.

Note that since μ depends on λ , for each λ the prescription chooses a different initial state in sLQC $_{(\lambda)}$. If $\underline{\chi}(y)$ were peaked at some value y_o , each $F_{(\lambda)}(x)$ will also be peaked at some x_o . However, as λ decreases this peak would shift progressively to $x = -\infty$. This change of the functional form of $F_{(\lambda)}(x)$ with λ is the ‘renormalization flow’ required to ensure that physics of the initial state remains the same at each scale λ .

Let us now evolve these states. Since $\hat{p}_{(\phi)}$ is a constant of motion, the non-trivial dynamics is in the expectation values of the volume operator. (4.7) immediately implies that while the difference between the two sets of expectation values will in fact shrink as ϕ increases, in the distant past it will grow unboundedly! Thus, the two sets of dynamics approximate each other well only on a semi infinite time interval (which is finite in the negative ϕ direction).

What happens when we shrink λ ? Since

$$V_- = \frac{4\pi\gamma\ell_{\text{Pl}}^2\lambda}{\sqrt{12\pi G}} \left[\int_{-\infty}^{\infty} dx \left| \frac{dF}{dx} \right|^2 e^{\sqrt{12\pi G}x} \right], \quad (4.10)$$

and since $F_{(\lambda)}(x) = \underline{\chi}(x + \mu)$ where μ monotonically decreases and $\mu \rightarrow -\infty$ as $\lambda \rightarrow 0$, V_- decreases steadily in this limit. Therefore, it follows from (4.2) that the condition $|\langle \hat{V} |_{\phi} \rangle_{\text{wdw}}(\phi) - \langle \hat{V} |_{\phi} \rangle_{(\lambda)}(\phi)| < \epsilon$ is satisfied further and further in the distant past. Therefore, given an $\epsilon > 0$ and *any* semi-infinite time interval $I = (-\phi_o, \infty)$, *however large ϕ_o may be*, there exists a $\lambda > 0$ such that the dynamical evolution of $\langle \hat{V} \rangle$ in sLQC $_{(\lambda)}$ dynamics remains within ϵ of that in the WDW theory on I . In particular, as observed in [3], as we shrink λ , for the same initial data at $\phi = 0$, the bounce time ϕ_{B} is pushed further and further into the past.

To summarize, the LQC dynamics does *not* reduce to the WDW dynamics as the area gap shrinks to zero. However, if one is interested only in semi-infinite intervals such as $(-\phi_o, \infty)$, one can recover the WDW dynamics on choosing *by hand* a sufficiently small λ .

V. TWO STRIKING FEATURES OF SLQC

This section is divided into two parts. In the first, we show that matter density admits an absolute upper bound ρ_{sup} on the physical Hilbert space which, furthermore, equals the critical density ρ_{crit} found in [3, 4] using effective equations and numerical evolutions of the exact equations. In the second, we show that there is a precise sense in which sLQC is a fundamentally discrete theory.

A. An absolute upper bound on matter density

The fact that *every* LQC physical state undergoes a bounce at a positive value of $\langle \hat{V} |_{\phi_B} \rangle$ provides a sense in which the singularity is resolved in LQC. We will now show that there is a much stronger sense in which the resolution occurs: the spectrum of the density operator $\hat{\rho}|_\phi$ is bounded above on the full physical Hilbert space \mathcal{H}_{phy} . Note that the boundedness of volume by itself is *not* sufficient to imply the boundedness of $\hat{\rho}|_\phi$ *because the operator $\hat{p}_{(\phi)}$ does not have a finite upper bound on \mathcal{H}_{phy} .*

In the classical theory, the scalar field density is given by $\rho|_\phi = (1/2)(p_{(\phi)}/V|_\phi)^2$. Since the operators $\hat{p}_{(\phi)}$ and $\hat{V}|_\phi$ do not commute in quantum theory, it is natural to define the density operator as

$$\hat{\rho}|_\phi = \frac{1}{2} \hat{A}|_\phi^2 \quad \text{where} \quad \hat{A}|_\phi = (\hat{V}|_\phi)^{-1/2} \hat{p}_{(\phi)} (\hat{V}|_\phi)^{-1/2} \quad (5.1)$$

Now, because $\hat{p}_{(\phi)}$ is a constant of motion, in any given physical state one would expect the time-dependent observable $\hat{\rho}|_\phi$ to reach its maximum value ρ_B at internal time $\phi = \phi_B$. Numerical simulations have shown [3, 4] that for states which are semi-classical at late times the value of ρ_B is remarkably robust: $\rho_B \approx 0.41\rho_{\text{Pl}}$ for all the states considered in models with and without a cosmological constant and also for the $k = \pm 1$ cosmologies. (It was therefore called critical density and denoted ρ_{crit}). It is natural to ask if this fact has an analytical explanation in sLQC. We will now show that the answer is in the affirmative.

Let us first compute the expectation values of the operator \hat{A} using those of $\hat{p}_{(\phi)}$ and $\hat{v}|_\phi$ given in (3.18)

$$\begin{aligned} \langle \hat{A} \rangle &:= \frac{(\Psi, \hat{A}|_{\phi_o} \Psi)_{\text{phy}}}{(\Psi, \Psi)_{\text{phy}}} = \frac{(\chi, \hat{p}_{(\phi)} \chi)_{\text{phy}}}{(\chi, \hat{V}|_{\phi_o} \chi)_{\text{phy}}} \\ &= \left(\frac{3}{4\pi\gamma^2 G} \right)^{\frac{1}{2}} \frac{1}{\lambda} \frac{\left[\int_{-\infty}^{\infty} dx |\partial_x F|^2 \right]}{\left[\int_{-\infty}^{\infty} dx |\partial_x F|^2 \cosh(\sqrt{12\pi G} x) \right]} \end{aligned} \quad (5.2)$$

where

$$\chi(x, \phi) = \hat{V}^{-\frac{1}{2}} \Psi = \frac{1}{\sqrt{2}} (F(x_+) - F(x_-)) \quad (5.3)$$

and the integrals are performed at $\phi = \phi_o$. Since $\cosh(\sqrt{12\pi G} x) \geq 1$, it follows that the ratio of the two integrals is bounded above by 1. Therefore, using the fact that $\lambda^2 = 2\sqrt{3}\gamma\ell_{\text{Pl}}^2$ in LQC, we obtain

$$\langle \hat{A} \rangle \leq \left(\frac{3}{4\pi\gamma^2 G} \right)^{\frac{1}{2}} \frac{1}{\lambda} \quad (5.4)$$

This implies that the spectrum of $\hat{A}|_\phi$ is bounded above by the right side of (5.4). Therefore the spectrum of $\hat{\rho}|_\phi = \hat{A}^2|_\phi$ is also bounded by

$$\rho_{\text{sup}} = \frac{3}{8\pi\gamma^2 G} \frac{1}{\lambda^2} = \frac{\sqrt{3}}{32\pi^2\gamma^3 G^2 \hbar} \approx 0.41\rho_{\text{Pl}}, \quad (5.5)$$

where in the last step we have used the value $\gamma \approx 0.24$ for the Barbero-Immirzi parameter that led to $\rho_{\text{crit}} \approx 0.41\rho_{\text{Pl}}$ in [3, 4, 14]. We wish to emphasize that this is an absolute bound on the spectrum of $\hat{\rho}|_\phi$ on the entire physical Hilbert space \mathcal{H}_{phy} ; there is no restriction that the states be, e.g., semi-classical. Note also that a factor of 10 in the value of γ would change ρ_{sup} (and ρ_{crit}) by a factor of 10^3 . The fact that the value of γ obtained from the entropy calculation yields $\rho_{\text{sup}} \sim \rho_{\text{Pl}}$ points to an overall coherence of LQG.

Finally, we could also have defined, as a measure of mean density, the quantity $\tilde{\rho} = \langle \hat{p}_{(\phi)} \rangle^2 / 2 \langle \hat{V}|_\phi \rangle^2$. It is easy to verify using the reasoning that led us to (5.5) that $\tilde{\rho}$ is also bounded above by ρ_{sup} .

Two questions arise immediately: Is this supremum attained? And, how does it relate to the upper bound ρ_{B} on density *along individual dynamical trajectories*? The fact that the value of ρ_{sup} is the same as ρ_{crit} suggests that the answers to the two questions are related. This is indeed the case.

Let $\tilde{F}(k)$ be a smooth function satisfying the following conditions:

$$\tilde{F}(k) = \frac{1}{k} e^{-\frac{\beta^2(k-k_o)^2}{2}} e^{ikx_o} \text{ if } k > \epsilon\sqrt{G} > 0 \quad \text{and} \quad \tilde{F}(k) = 0 \text{ if } k \leq 0, \quad (5.6)$$

where $\epsilon \ll 1 \ll k_o/\sqrt{G}$. This is a semi-classical initial state peaked at $k = k_o$ and $x = x_o$. Let $F(x)$ be its Fourier transform. Then $\chi(x, \phi) = (1/\sqrt{2})(F(x_+) - F(x_-))$ is a physical state. One can readily calculate the expectation values $\langle \hat{p}_{(\phi)} \rangle$ and $\langle \hat{V}|_\phi \rangle$ in this state. Since $\langle \hat{p}_{(\phi)} \rangle$ is a constant of motion and $\langle \hat{V}|_\phi \rangle$ attains its minimum, V_{B} , at the bounce point, as expected ρ attains its maximum also at the bounce point. It is given by:

$$\rho_{\text{B}} = \rho_{\text{sup}} \left[1 - O \left(\frac{G\hbar^2}{p_{(\phi)}^2 + (\Delta p_{(\phi)})^2} \right) \right] \quad (5.7)$$

where we have used the fact that $\Delta p_{(\phi)} = \hbar\beta$.

Thus, for semi-classical states ρ_{B} is very close to ρ_{sup} . Typical numerical simulations of [3] used such semi-classical states with $\langle \hat{p}_{(\phi)} \rangle = 5 \times 10^3 \hbar$ (in the classical units $G = c = 1$) with the relative dispersion $\Delta p_{(\phi)} / \langle \hat{p}_{(\phi)} \rangle$ of 2.5%. In this case, the above calculation shows that $\rho_{\text{sup}} - \rho_{\text{B}} = O(10^{-4})$, whence the value $\rho_{\text{crit}} = 0.41\rho_{\text{Pl}}$ of that numerical simulation is consistent with the above analytical calculation in the simplified model. Note incidentally that even this state represents a universe that is very quantum mechanical. In the $k = 1$ case for example, a state with these parameters represents a universe which grows to a *maximum* radius of only $\sim 25\ell_{\text{Pl}}$ before undergoing a classical recollapse. If we use values of $\langle \hat{p}_{(\phi)} \rangle$ and $\Delta p_{(\phi)}$ that correspond to universes that grow, say a megaparsec size in the $k = 1$ case [4], ρ_{sup} would agree to ρ_{B} to 1 part in 10^{230} . These considerations show that on \mathcal{H}_{phy} , ρ_{B} can come arbitrarily close to ρ_{sup} .

B. Fundamental discreteness of sLQC

We saw in section IV B that the WDW dynamics does not result in the limit $\lambda \rightarrow 0$ of $\text{sLQC}_{(\lambda)}$. A natural question then is whether $\text{sLQC}_{(\lambda)}$ admits any limit at all as the area

gap shrinks to zero. We will now show that the answer is in the negative. The underlying conceptual idea is simple: the one-parameter family of theories $\text{sLQC}_{(\lambda)}$ will admit a limit as $\lambda \rightarrow 0$ if, given any $\epsilon > 0$ there exists a $\delta > 0$ such that the predictions of all $\text{sLQC}_{(\lambda)}$ with $\lambda < \delta$ agree within ϵ for all times ϕ . We will argue by contradiction.

Suppose then that the limit exists. Fix an ϵ and let $\lambda, \lambda' < \delta$. Fix a normalized state $\chi_{(\lambda)}$ in $\text{sLQC}_{(\lambda)}$. Then by assumption $\text{sLQC}_{(\lambda')}$ admits a normalized state $\chi_{(\lambda')}$ which is ‘close’ to it. In particular then,

$$|\langle \hat{V} | \phi \rangle_{(\lambda)} - \langle \hat{V} | \phi \rangle_{(\lambda')}| < \epsilon, \quad (5.8)$$

and, to keep transparency of equations we will assume that $\langle \hat{p}_{(\phi)} \rangle_{(\lambda)} = \langle \hat{p}_{(\phi)} \rangle_{(\lambda')}$.¹⁰ Now, since

$$\langle \hat{V} | \phi \rangle_{(\lambda)} = V_+(\lambda)e^{\sqrt{12\pi G}\phi} + V_-(\lambda)e^{-\sqrt{12\pi G}\phi}, \quad (5.9)$$

Eq (5.8) can be satisfied for all ϕ if and only if the $V_{\pm}(\lambda) = V_{\pm}(\lambda')$. It then follows from (4.4) that the densities at the bounce points of the two theories are equal:

$$\rho_B(\lambda) = \frac{1}{8} \frac{\langle \hat{p}_{(\phi)} \rangle^2}{V_+(\lambda)V_-(\lambda)} = \frac{1}{8} \frac{\langle \hat{p}_{(\phi)} \rangle^2}{V_+(\lambda')V_-(\lambda')} = \rho_B(\lambda'). \quad (5.10)$$

Now fix $\lambda' < \delta$, choose $\lambda = \lambda'/N$ for some $N > 1$ and let $\chi_{(\lambda)}$ be a semi-classical state with $\rho_B(\lambda) = \rho_{\text{sup}}(\lambda) - \tilde{\epsilon}$. As we saw in section V A, we can choose $\chi_{(\lambda)}$ so that $\tilde{\epsilon}$ is arbitrarily small. But then (5.10) and (5.5) imply

$$\rho_B(\lambda') = \rho_B(\lambda) = \rho_{\text{sup}}(\lambda) - \tilde{\epsilon} = N^2 \rho_{\text{sup}}(\lambda') - \tilde{\epsilon} > \rho_{\text{sup}}(\lambda') \quad (5.11)$$

if we choose N to be sufficiently large. But this is impossible since $\rho_{\text{sup}}(\lambda')$ is an absolute upper bound on density in the physical Hilbert space of the $\text{sLQC}_{(\lambda')}$ theory. This implies that our initial assumption that the limit exists is invalid. sLQC does not admit a continuum limit; it is a fundamentally discrete theory. This establishes the main result of this section.

It is useful to note that, by replacing $b_o\lambda$ with λ/λ' in (4.9), the procedure introduced in section IV B leads to a rather natural ‘renormalization flow’ relating states of the 1-parameter family of $\text{sLQC}_{(\lambda)}$ theories. Under this flow, if the initial $\chi_{(\lambda)}(x)$ is semi-classical in $\text{sLQC}_{(\lambda)}$, the state $\chi_{(\lambda')}(x)$ will also be semi-classical in $\text{sLQC}_{(\lambda')}$. The classical trajectories on which the two states are peaked in the future will be very close to one another. Each state will also remain peaked on a classical trajectory in the (pre-bounce) distant past. However, these two classical trajectories will be very different and diverge away from each other in the past evolution. Thus, while there is a bounce in each $\text{sLQC}_{(\lambda)}$, the pre-bounce dynamics is vastly different for different values of λ .

The non-convergence of sLQC in the $\lambda \rightarrow 0$ limit shows that sLQC is qualitatively different from polymer quantum mechanics [16–18] and lattice gauge theories. The polymer particle example was introduced as a toy model to probe certain mathematical and conceptual issues and by itself does not have direct physical significance. While it has certain similarities with LQC, there are also important differences. Because there is no positive

¹⁰ It is completely straightforward to extend the argument to allow these expectation values to be different but within ϵ of each other. Requiring an exact equality is also motivated by the fact that $p_{(\phi)}$ is a constant of motion and, even within a single $\text{sLQC}_{(\lambda)}$ theory, semi-classical states with different values of $p_{(\phi)}$ depart from each other unboundedly under evolution.

frequency requirement in the polymer particle theory, the physical inner product and the Hamiltonian are local. Arguments that are successful in that example simply break down because of non-locality of sLQC. Lattice gauge theories are meant to be controlled approximations to the continuum theory. As in numerical analysis of PDEs, the discreteness is introduced just as an intermediate mathematical simplification. Therefore, absence of a continuum limit would be tantamount to non-viability of that theory. In LQG on the other hand the continuum is only an approximation. Not only is there no a priori reason for the theory to make sense as the area gap is shrunk to zero, but within the LQG framework it would be hard to make physical sense of the limit if it existed. Discreteness at the Planck scale is a fundamental and essential ingredient of the theory. The continuum emerges on coarse graining; ignoring the fine structure of quantum geometry because one is not interested in phenomena at the Planck scale is very different from taking the naive continuum limit $\lambda \rightarrow 0$ which corresponds to washing out quantum geometry at all scales.

VI. DISCUSSION

Detailed analysis of the physical sector of LQC has revealed that the older quantum Hamiltonian constraints [10, 11] have serious drawbacks already in the FRW models coupled to at least one massless scalar field [2]. In particular, they lead to physically unacceptable breakdown of general relativity in completely ‘tame’ regimes. The ‘improved’ constraint operator of [3] is free of these drawbacks. Within the FRW models, this improvement is robust in the sense that it extends to situations in which there is a non-zero cosmological constant and/or non-zero spatial curvature corresponding to the $k=1$ cosmologies [3, 4]. Recent analysis has shown that its bounce picture is also robust with respect to the inclusion of a phenomenologically viable inflationary potential [32]. Thus, the suggestion (see, e.g., [13, 15]) that the bounce would not persist once a potential is included has turned out to be incorrect.

However, so far predictions from ‘improved’ dynamics were all made numerically using states which are semi-classical at late times. Three somewhat different classes of semi-classical states were used and numerical simulations were carried out in two distinct ways, using a variety of values of the parameters involved. While these features had established a certain degree of robustness of results, in absence of an analytical understanding of dynamics, it was not obvious whether the results would continue to hold for generic states. Indeed, it has been suggested that they may not [15] and concerns have been expressed that numerical subtleties may affect the robustness of the bounce [31].

In this paper we obtained an analytically soluble model —sLQC— by adapting the theory to the scalar field clock already at the classical level. This allows one to consider generic states and analyze physics without recourse to any numerics. The question then is: Does the quantum bounce persist generically and, if so, does it continue to be approximately symmetric about the bounce point? Or, are these features restricted just to semi-classical states? A natural avenue to explore these questions is through dynamics of the expectation values of the volume operator. We found that these undergo a quantum bounce for *all* states and furthermore the bounce continues to be symmetric. Thus the bounce and its salient qualitative feature are quite robust in the cosmological model under consideration. More importantly, we could show that matter density has an absolute supremum ρ_{sup} on the physical Hilbert space, given by: $\rho_{\text{sup}} = \sqrt{3}/32\pi^2\gamma^3 G^2 \hbar \approx 0.41\rho_{\text{Pl}}$. This is precisely the value of the critical density ρ_{crit} [3, 4] at which the bounce occurs in numerical simulations

and in solutions to effective equations, both of which are, however, based on states that are semi-classical at late times. Thus the *raison d'être* and the observed robustness of the somewhat mysterious ρ_{crit} was clarified analytically.

We could also use the model to analyze the relation between the WDW theory and sLQC. It is well known that the key differences between the two theories can be traced back to the fact that dynamics of LQC incorporates the quantum nature of geometry through the area gap $\Delta \ell_{\text{Pl}}^2$. The question then is: Can one regard the WDW theory as the limit of LQC when quantum geometry effects are ignored by taking the mathematical limit $\Delta \rightarrow 0$? Since it is analytically soluble, sLQC is well suited to probe this issue. We used the complete set of Dirac observables, $\hat{p}_{(\phi)}, \hat{V}|_{\phi}$ to compare the two theories and obtained two results. First, suppose we fix any semi-infinite interval I of internal time and an $\epsilon > 0$. Then one *can* approximate sLQC by the WDW theory to within ϵ over the time interval I simply by shrinking by hand the area gap sufficiently. In this sense the answer to the question is in the affirmative. However, if one is interested in the *global* time evolution —i.e., if we let I be the full real line— then the answer is in the negative: No matter how much we shrink the area gap, if we wait long enough the difference in the predictions of the two theories will become as large as we want. Furthermore, in terms of global behavior in time, sLQC fails to admit any well-defined limit as the area gap shrinks to zero. In this sense sLQC is a fundamentally discrete theory. The use of a non-zero Δ in LQC is not just an intermediate step to make the quantum theory mathematically manageable. Rather, the presence of a non-zero area gap is a central physical feature of LQC, an imprint of the quantum geometry of full LQG on this symmetry reduced theory. The dramatic difference from the more familiar lattice gauge theories is that whereas QCD can be meaningfully formulated in the continuum, quantum general relativity cannot; in LQG it is essential to use quantum geometry at the Planck scale.

We wish to emphasize, however, that the analysis of this paper has two main limitations. First, we restricted ourselves to the simplest model, the $k=0$ FRW cosmology coupled to a massless scalar field. The robustness refers to states within this model (although most results can be probably generalized by including a cosmological constant or allowing the $k=1$ closed models). The second and much more important limitation is that as of now LQC has *not* been systematically derived from LQG. In the LQC Hamiltonian constraint, the area gap enters through the definition of the field strength F_{ab}^i via holonomies of the gravitational connection A_a^i . This strategy is standard in full LQG. However, in LQC one breaks diffeomorphism invariance through gauge fixing. While this is the standard practice in all approaches to (classical and) quantum cosmology, it implies that we cannot directly employ the full strategy used so far in LQG. The new element —which may also be useful in a suitably gauge fixed version of full LQG— is that the loop along which the holonomy is defined is shrunk not to zero but only till it encloses an area a_o of Planck size. Now the most natural value of a_o is the smallest non-zero area eigenvalue $\Delta \ell_{\text{Pl}}^2$ in the class of states relevant to LQC, called the area gap. However, in this step one parachutes by hand a result from full LQG into LQC. This is analogous to the procedure used in the Bohr atom where one puts in the quantization $j = n\hbar$ of angular momentum by hand. In retrospect, this step is parachuted from the more complete quantum mechanics. However, a fuller understanding shows that while angular momentum is indeed quantized, its eigenvalues are $\sqrt{j(j+1)}\hbar$ rather than $n\hbar$. In a similar vein the quantization of area is parachuted into LQC from the more complete theory of quantum geometry in LQG. We believe that this step will be eventually justified through a systematic derivation of LQC from LQG. However, just as the

correct eigenvalues of angular momentum are more subtle than the ‘natural’ or ‘obvious’ values $n\hbar$ used in the Bohr atom, the correct value of the area a_o to which the holonomy loops have to be shrunk may have a value different from $\Delta \ell_{\text{Pl}}^2$. For instance, arriving at LQC from LQG may well require a coarse graining which could lead to a ‘dressing’ of Δ .

We will conclude by comparing and contrasting our model with another soluble model that has recently appeared in the literature also for the $k = 0$ cosmology with a massless scalar field [15]. There, in essence one begins with a classical constraint, $c^2 p^2 = \text{const } p_{(\phi)}^2$, takes its positive square root and quantizes by replacing c by $\sin c$ and p by $-i\hbar\partial_c$. Thus one first simplifies the *classical* constraint and then quantizes, using rules motivated by LQC.¹¹ By contrast, in this paper started with the lapse function suited to harmonic rather than proper time but then followed the same procedure as in [3] to obtain the improved *quantum* constraint. Therefore, reservations [15] that the simplified model may leave out interesting physics are inapplicable for the model discussed in this paper. At least for the $k=0$ FRW models with a massless scalar field, the bounce scenario that emerged from numerical simulations in [3] appears to be robust, i.e., is not tied to states which are semi-classical at late times.

Finally, there are three other key differences between the two exactly soluble models. First, the simplified constraint used in [15] corresponds to a difference equation with uniform steps in $p \sim a^2$ rather than in volume ($\sim a^3$). Therefore, it is the analog of the older Hamiltonian constraint [10, 11] used in LQC which, as we discussed in sections I and III A, leads to physically unacceptable predictions. Second, simplifications of [15] removes, by hand, the right or the left moving sector of the theory. This truncation is motivated by considerations of mathematical simplicity but does not appear to have any physical justification. Third, as in LQC, the ‘evolution equation’ satisfied by physical states in our simplified model involves the square-root of a positive operator (Θ) and is thus fundamentally non-local. This is a direct consequence of the group averaging procedure used to obtain the physical Hilbert space. By contrast, because the square-root of the constraint is taken classically in [15], the resulting operator is local (in c) unlike the corresponding operator in full LQC [3]. In the terminology of section III, while the physical states of the model discussed in this paper have only ‘positive frequency’ modes but with both right and left moving components, those of [15] contain both positive and negative frequency modes but restricted to be either left or right moving.

The simplified model introduced in this paper will be used in [19] also to analyze properties of fluctuations in volume. Again it will turn out that indications provided by numerical simulations involving states which are semi-classical at late times [3] are realized by generic states.

¹¹ The replacement $c \rightarrow \sin c$ is motivated by the older, ‘ μ_o quantization’ of LQC [2, 10, 11] but with μ_o set to 1. However, since it is just c rather than c^2 that now appears in the square root of the classical constraint, it cannot be directly related to the field strength F_{ab}^i , whence the replacement $c \rightarrow \sin c$ no longer ‘descends’ from LQG. See the remark at the end of section III.

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Appendix A: Starting with harmonic versus proper time already in the classical theory

In the ‘improved’ dynamics of [3], one began with proper time in the classical theory (where the lapse is given by $N = 1$) and switched to the scalar field time only after obtaining the quantum Hamiltonian constraint. In section III by contrast we first adapted the classical theory to the scalar field time (by using $N = a^3$) and then proceeded with quantization. The two strategies yield slightly different factor orderings in the quantum Hamiltonian constraint. In this Appendix we will discuss the detailed relation between them. It will turn out that the difference is negligible on physical grounds.

If one begins with the lapse $N = 1$ and then passes to quantum theory, the gravitational part of the ‘improved’ Hamiltonian is given by (see Eqs. (2.23)-(2.25) of [3]):

$$\hat{C}_{\text{grav}} \tilde{\Psi}(\nu, \phi) = (\sin \lambda b) A(\nu) (\sin \lambda b) \tilde{\Psi}(\nu, \phi) \quad (\text{A1})$$

with

$$A(\nu) = -\frac{6\pi\ell_{\text{Pl}}^2}{\gamma\lambda^3} |\nu| \left| |\nu + \lambda| - |\nu - \lambda| \right|, \quad (\text{A2})$$

where $\lambda > 0$ is given by $\lambda^2 = \Delta \ell_{\text{Pl}}^2 \equiv 2\sqrt{3}\pi\gamma \ell_{\text{Pl}}^2$. The matter part of the Hamiltonian constraint is given by:

$$\hat{C}_{\text{matt}} \tilde{\Psi}(\nu, \phi) = 8\pi G \hat{p}_{(\phi)}^2 \widehat{V}^{-1} \tilde{\Psi}(\nu, \phi). \quad (\text{A3})$$

Using the Thiemann strategy, [25, 26], we can calculate the operator \widehat{V}^{-1} in the ν -representation. As expected, this operator is diagonal:

$$\begin{aligned} \widehat{V}^{-1} \tilde{\Psi}(\nu) &= \frac{27}{64} \frac{1}{\lambda^3 \alpha} \left| |\nu + \lambda|^{\frac{2}{3}} - |\nu - \lambda|^{\frac{2}{3}} \right|^3 \tilde{\Psi}(\nu, \phi) \\ &=: B(\nu) \tilde{\Psi}(\nu, \phi). \end{aligned} \quad (\text{A4})$$

Thus, if one begins with $N = 1$ in the classical theory, the Hamiltonian constraint is given by

$$\partial_\phi^2 \tilde{\Psi}(\nu, \phi) = \frac{1}{8\pi G \hbar^2} B^{-1}(\nu) \sin \lambda b A(\nu) \sin \lambda b \tilde{\Psi}(\nu, \phi) \quad (\text{A5})$$

The key difference from the constraint (3.7) used in the main text is that in (3.7) each of the functions $A(\nu)$ and $(B(\nu))^{-1}$ is replaced by (certain multiples of) $|\nu|$.

The question then is: Under what conditions does (A5) reduce to (3.7)? Note first that in the main text we restricted ourselves to the lattice $\nu = 4n\lambda = 4n\sqrt{\Delta}\ell_{\text{Pl}}$. On the points of this lattice, we have $A(\nu) = -(12\pi\ell_{\text{Pl}}^2/\gamma\lambda^2)|\nu|$. For $B(\nu)$ let us make a weak assumption:

- *Let us replace $B(\nu)$ with its WDW value $(2\pi\gamma\ell_{\text{Pl}}^2|\nu|)^{-1}$. This amounts to assuming $O(|\lambda/\nu|) \ll 1$. Now, because of the form of the inner product, the state $|\nu\rangle = 0$ on which the approximation would have been the worst does not feature in the physical Hilbert space of [3] nor in the physical Hilbert space used in the main text. As figure 1 shows the ‘error’ is only 1.43% for $\nu = 4\lambda$, 0.02% for $\nu = 8\lambda$ and decreases extremely rapidly for higher ν .*

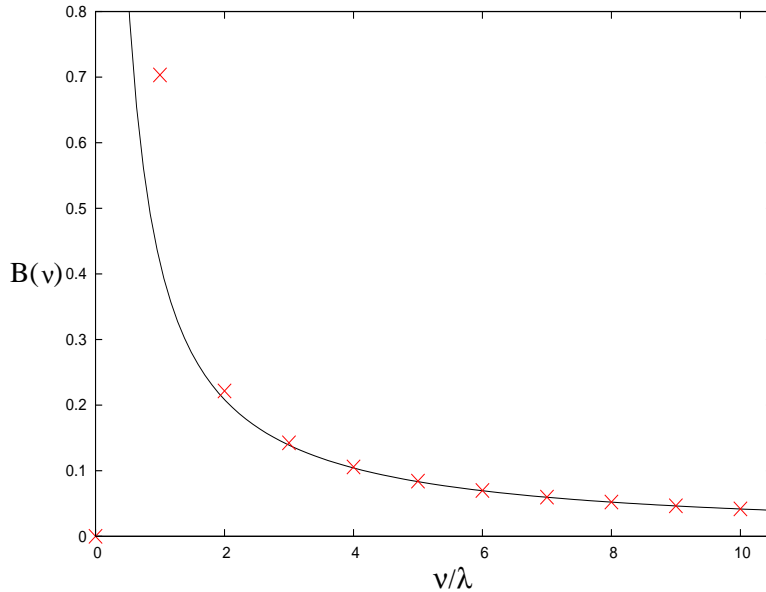


FIG. 1: Crosses denote values of the LQC function $B(\nu)$ for $\nu/\lambda = n$. The continuous curve represents the sLQC approximation used in this paper. Physically relevant points are $\nu/\lambda = 4n$ with $n \geq 1$. The relative ‘error’ is 1.43% for $n = 1$, 0.02% for $n = 2$ and further decreases extremely rapidly for higher n .

With this simplification¹², the total constraint $(\hat{C}_{\text{grav}} + \hat{C}_{\text{matt}})\tilde{\Psi} = 0$ takes the form

$$\partial_\phi^2 \tilde{\Psi}(\nu, \phi) = 3\pi G |\nu| \frac{\sin \lambda \mathbf{b}}{\lambda} |\nu| \frac{\sin \lambda \mathbf{b}}{\lambda} \tilde{\Psi}(\nu, \phi) \quad (\text{A6})$$

which is precisely the constraint (3.8) used in the main text. To summarize, mathematically the Hamiltonian constraint of [3] reduces to the one used in the main text if one replaces $B(\nu)$ in [3] by its WDW value. The difference between the two constraint is less than 2% even for the state concentrated at $\nu = 4\lambda$ and decreases extremely rapidly for states with support at higher values of ν .

¹² In [29] properties of the Hamiltonian constraint of [3] were established using a procedure which began precisely with our simplified operator. That analysis also provides a systematic leading order correction to the ‘simplification’ made here.

Finally, it is natural to ask if the simplifying assumption on $B(\nu)$ is violated near the bounce point. If the violation is significant, then the conclusions drawn from the solvable model could be qualitatively different from those drawn from the constraint used in [3]. Now, since in the ν representation *physical* states have support only on points $\nu = 4n\lambda$ with $|n| > 0$, it follows that V_{\min} is necessarily bounded below by $8\pi\gamma\ell_{\text{Pl}}^2\lambda$. This value is in fact attained by the physical state $\tilde{\chi}(\nu, \phi) = (\exp i\sqrt{\Theta}\phi) \delta_{|n|,1}$ in the ν -representation, or, $\chi(x, \phi) = (\exp i\sqrt{\Theta}\phi) \sin(4 \arctan \sqrt{12\pi G}x)$ in the x representation. In this state, the expectation value $\langle \hat{p}_{(\phi)} \rangle$ of the constant of motion $\hat{p}_{(\phi)}$ is $\sim \hbar$ (in the classical units $G=c=1$). Therefore this state belongs to the extreme quantum regime. For example, in the case of $k=1$, closed universes, classical Einstein's equations imply that a universe with such a value of $p_{(\phi)}$ can expand out to a *maximum* radius only of $\sim 0.3\ell_{\text{Pl}}$ before recollapsing to a big-crunch. Even for such an extreme quantum state, the treatment of the main text is close to that in [3]: as figure 1 shows, for $B(\nu)$ the relative error is $\sim 1.4\%$. In any state which can be thought of as representing a classical universe at late times even in a very weak sense, the difference between the two factor orderings would be further suppressed by an enormous factor.

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