

Isotropic loop quantum cosmology with matter

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A free massless scalar field is coupled to homogeneous and isotropic loop quantum cosmology. The coupled model is investigated in the vicinity of the classical singularity, where discreteness is essential and where the quantum model is nonsingular, as well as in the regime of large volumes, where it displays the expected semiclassical features. The particular matter content (massless, free scalar) is chosen to illustrate how the discrete structure regulates pathological behavior caused by kinetic terms of matter Hamiltonians (which in standard quantum cosmology leads to wave functions with an infinite number of oscillations near the classical singularity). Because of this modification of the small volume behavior the dynamical initial conditions of loop quantum cosmology are seen to provide a meaningful generalization of DeWitt's initial condition.

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I. INTRODUCTION

Since the early days of canonical quantum gravity [1,2] isotropic cosmological models have been popular test objects. In the geometrodynamical approach quantum states are considered to be continuous functions of one or more variables, typically metric or extrinsic curvature quantities of space-like slices, and of matter variables if the system is coupled to matter. Whereas in general geometrodynamics the configuration space for wave functions is the “superspace of geometries” with infinitely many degrees of freedom parametrizing the metric at each point of space, the number of degrees of freedom of homogenous models reduces to a finite amount since all geometric quantities are spatially constant. Such “mini-superspace” models thus become accessible to quantum mechanical methods, while one has to be careful when interpreting the results in light of the strong reduction of the number of degrees of freedom. The isotropic model represents the smallest possible minisuperspace with only one geometric degree of freedom, the radius of the universe.

In the classical limit at large volume such models are well behaved and reproduce their classical counterpart. The problem of the classical singularity at zero volume, however, is not cured, which is related to the fact that spectra of geometric operators remain continuous in standard quantum cosmology. (Nevertheless, at the level of *expectation values* the expansion or contraction velocity, for example, may remain finite and discrete features may emerge [3].) On the other hand, loop quantum cosmology [4] inherits from quantum geometry a discrete structure of geometry [5,6] which is most relevant at small scales. Still, at large volume standard

quantum cosmology emerges as an approximation [7] which is very good in the semiclassical regime but not applicable near the classical singularity, where quantum effects of gravity become dominant and the discreteness of geometry at the scale of the Planck length becomes essential. The discreteness leads to a resolution of the singularity problem through the following mechanism: Already at the kinematical level, there is an indication for a natural curvature cutoff since the classically diverging quantity a^{-1} has a finite quantization with an upper bound of the size of the inverse Planck length [8]. Furthermore, an investigation of the dynamical evolution confirms that the classical singularity does not appear as a boundary but instead allows a well-defined evolution through it [9].

In the context of the present paper we are mostly interested in another consequence of loop quantum cosmology: namely, that it predicts dynamical initial conditions which are derived from the evolution equation [10]. The issue of initial conditions in quantum cosmology has been widely discussed [1,11,12], in part as an attempt to deal with the singularity. DeWitt's initial condition, which is closely related to the outcome of the dynamical initial conditions, requires the wave function to vanish at the classical singularity (which, however, with continuous geometrical spectra does not solve the singularity problem since one can still get arbitrarily close to vanishing volume [14]). On the other hand, it is well known that DeWitt's condition is not applicable in general because in most cases it would predict an identically vanishing wave function. A particularly thorny issue, also for other boundary proposals, is the fact that solutions to the Wheeler-DeWitt equation often exhibit an infinite number of oscillations between the vanishing scale factor and any finite value. In such a case, the limit of the wave function for $a \rightarrow 0$ is not always well defined and one cannot even impose initial conditions at $a=0$. The origin of the infinite number of oscillations is the kinetic term in a matter Hamiltonian

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which is proportional to a^{-3} . At small a , the Wheeler-DeWitt equation requires the derivative of the wave function to be proportional to the square root of the kinetic term, which diverges for $a \rightarrow 0$. Usually, one tries to avoid this problem by choosing a wave function which is independent of the matter field at small a so that the matter momentum vanishes and the kinetic term is identically zero. However, for larger volume the wave function *must* depend on the matter field non-trivially which forces a dependence at small volume, too. Even if the dependence is only weak, the diverging kinetic term will eventually dominate when a is small enough. In the present paper we investigate if there is a more natural way to deal with this problem from the point of view of loop quantum cosmology.

Since this problem is caused by the kinetic term independently of the potential, we will analyze it in the most simple setting, which is isotropic loop quantum cosmology coupled to a free massless scalar field. In this way, the total quantum Hamiltonian acts on the state function containing one degree of freedom of geometry and one of matter. The formulation is based on [4,8] where a discrete orthonormal basis of states of homogeneous and isotropic quantum geometry has been established which provides eigenstates of the volume operator.

This paper is organized as follows. In Sec. II the quantum Hamiltonian constraint equation with a massless scalar field is formulated, leading to a difference equation which is solved in Sec. III. In Sec. IV the continuum and semiclassical limit are considered and possible physical consequences are discussed. Section V deals with a comparison of different proposals for initial conditions.

II. THE QUANTUM HAMILTONIAN CONSTRAINT

We begin with the Lagrange density of a massless scalar field ϕ on a spacelike slice of a canonically decomposed 4-dimensional space-time manifold,

$$\mathcal{L}_\phi = \frac{1}{2} [\dot{\phi}^2 - (\nabla \phi)^2],$$

where ∇ denotes the spatial derivative on the slice and the dot the derivative with respect to the time coordinate. In our case, the spatially flat Friedmann model with the metric

$$ds^2 = -dt^2 + a^2(t)[dx^2 + dy^2 + dz^2],$$

the total matter Lagrangian becomes

$$L_\phi = \int d^3x \sqrt{-g} \mathcal{L} = \frac{1}{2} \int d^3x a^3 \dot{\phi}^2,$$

where, in order not to disturb homogeneity, ϕ is assumed to be spatially constant so that the gradient term vanishes identically. The integral over the coordinate depending term, i.e. the total volume divided by a^3 , will be set equal to one which can be achieved by an appropriate compactification. For the Hamiltonian of the field we obtain

$$H_\phi = \frac{1}{2} p_\phi^2 a^{-3} \quad (1)$$

where $p_\phi = a^3 \dot{\phi}$ is conjugate to ϕ .

Together with the gravitational part of the Hamiltonian constraint [4] we obtain in the isotropic case

$$\begin{aligned} H &= -6\gamma^{-2}\kappa^{-1}c^2\sqrt{|p|} + H_\phi \\ &= -6\gamma^{-2}\kappa^{-1}c^2\sqrt{|p|} + \frac{1}{2}|p|^{-3/2}p_\phi^2 = 0 \end{aligned} \quad (2)$$

where the canonical gravitational degrees of freedom are the isotropic connection component c and (densitized) triad component p which fulfill $\{c, p\} = \frac{1}{3}\gamma\kappa$. Here, $\kappa = 8\pi G$ is the gravitational constant and γ the Barbero-Immirzi parameter [16] whose value does not affect the classical behavior (but it is important for the quantum theory since it scales the spectra of geometric operators). Because p is a triad component which has two possible orientations, it can take both positive and negative values. This is also true for the scale factor a which is the isotropic co-triad component and related to p by $p = \text{sgn}(a)a^2$. From now on, however, it will be sufficient to consider only positive p and a (though we keep absolute value signs in some formulas for the sake of generality). The connection component c is related to the extrinsic curvature and therefore to the time derivative of a by $c = \frac{1}{2}\dot{a}$.

In the absence of a potential, the matter momentum $p_\phi = \omega$ is a constant in time and the solution

$$c = \frac{1}{2}\gamma\sqrt{\kappa/3}\omega/p \quad (3)$$

of Eq. (2) only depends on p . To understand the classical evolution in a coordinate time t (with lapse function $N=1$) we compute

$$\dot{p} = \{p, H\} = 4\gamma^{-1}c\sqrt{p} = 2\sqrt{\kappa/3}\omega p^{-1/2}$$

yielding $p(t) = a(t)^2 = [\sqrt{3\kappa}\omega(t-t_0)]^{2/3}$, i.e. an eternally expanding universe.

Now we quantize the field canonically by assuming a wave function $\chi(\phi)$ and the canonical momentum acting as a derivative operator on it,

$$\hat{p}_\phi := -i\hbar \frac{d}{d\phi}, \quad (4)$$

so that the Hamiltonian for spatially constant fields becomes

$$\tilde{H}_\phi = -\frac{1}{2}\hbar^2|a|^{-3}\frac{d^2}{d\phi^2} \quad (5)$$

(it is denoted \tilde{H}_ϕ since we will later introduce another operator \hat{H}_ϕ in which a is also quantized).

For a quantization in the complete system of gravity and matter we need a quantization of the inverse power $|a|^{-3}$ which diverges classically close to the singularity. In standard quantum cosmology this would simply be quantized to a multiplication operator acting on wave functions depending on a , which does not cure the divergence. Loop quantum cosmology, on the other hand, can easily deal with this problem: while the volume operator has zero eigenvalues and so no well-defined inverse, there are well-defined quantizations

of inverse powers of the scale factor [8]. This inverse power of the scale factor is essential for the issues studied in the present paper. The details of the quantization of the matter field are irrelevant; one can also use quantization techniques inspired from loop quantum gravity (see e.g. [15]).

To specify the gravitational part of the wave function in loop quantum cosmology we start in the connection representation where an orthonormal basis is given by [4]

$$\langle c|n\rangle = \frac{\exp\left(\frac{1}{2}inc\right)}{\sqrt{2} \sin \frac{1}{2}c}, \quad n \in \mathbb{Z}. \quad (6)$$

A state $|n\rangle$ can be interpreted as an “isotropic spin network state” where $(|n|-1)/2$ plays the role of the spin label. As seen from the full theory, however, these states are distributional as a consequence of the symmetry and correspond to non-normalizable superpositions of ordinary spin network states. Still, the discrete structure of geometry is preserved when restricting to the states $|n\rangle$: They are eigenstates of the volume operator

$$\hat{V}|n\rangle = \left(\frac{1}{6} \gamma l_P^2\right)^{3/2} \sqrt{(|n|-1)|n|(|n|+1)} |n\rangle =: V_{(|n|-1)/2} |n\rangle \quad (7)$$

with discrete eigenvalues. If n is small the effects of the discreteness become most significant and there are departures from the classical geometry. For instance, there is a well-defined inverse scale factor operator which also has the states $|n\rangle$ as eigenstates and action (we only use the diagonal part of the operator \hat{m}_{IJ} derived in [7])

$$\widehat{|a|^{-1}}|n\rangle = 16(\gamma l_P^2)^{-2} (\sqrt{V_{|n|/2}} - \sqrt{V_{|n|/2-1}})^2 |n\rangle \quad (8)$$

with $l_P = \sqrt{\kappa \hbar}$ being the Planck length [in Eq. (8) V_{-1} is understood to be zero]. As discussed in [17], the quantization of the inverse scale factor is affected by quantization ambiguities. The effect of different choices will be discussed later; they do not lead to substantial changes in most of the following calculations and results.

The action of the gravitational Hamiltonian on the basis states $|n\rangle$ is [4,13]

$$\begin{aligned} \hat{H}_{\text{grav}}|n\rangle &= 3 \gamma^{-2} (\kappa \gamma l_P^2)^{-1} \text{sgn}(n) (V_{|n|/2} - V_{|n|/2-1}) \\ &\quad \times (|n+4\rangle - 2|n\rangle + |n-4\rangle). \end{aligned} \quad (9)$$

Now we write the states of the coupled system matter plus gravity as a superposition of geometry eigenstates

$$|s\rangle = \sum_{n=-\infty}^{\infty} s_n(\phi) |n\rangle \quad (10)$$

with ϕ -dependent coefficients $s_n(\phi)$ which represent the state in the triad representation. We use Eq. (8) to quantize the inverse volume in the matter Hamiltonian (5). Since the gravitational part of the resulting operator \hat{H}_ϕ is diagonal in the basis states $|n\rangle$ we can define

$$\hat{H}_\phi |n\rangle \otimes |\phi\rangle =: |n\rangle \otimes \hat{H}_\phi(n) |\phi\rangle \quad (11)$$

for each $|n\rangle$ and arbitrary $|\phi\rangle$. For the massless field we only have to insert the eigenvalue of $|a|^{-1}$ in a state $|n\rangle$, so we obtain

$$\hat{H}_\phi(n) = -\frac{1}{2} \hbar^2 16^3 (\gamma l_P^2)^{-6} (\sqrt{V_{|n|/2}} - \sqrt{V_{|n|/2-1}})^6 \frac{d^2}{d\phi^2}. \quad (12)$$

Finally, a state $|s\rangle$ is annihilated by the total Hamiltonian, the sum of \hat{H}_{grav} in (9) and \hat{H}_ϕ in Eq. (11) with Eq. (12), if s_n satisfies [we absorb the sign of n appearing in Eq. (9) into the wave function]

$$\begin{aligned} & (V_{|n+4|/2} - V_{|n+4|/2-1}) s_{n+4}(\phi) \\ & - 2(V_{|n|/2} - V_{|n|/2-1}) s_n(\phi) \\ & + (V_{|n-4|/2} - V_{|n-4|/2-1}) s_{n-4}(\phi) \\ & = \alpha \hbar^2 (\sqrt{V_{|n|/2}} - \sqrt{V_{|n|/2-1}})^6 \frac{d^2}{d\phi^2} s_n(\phi) \end{aligned} \quad (13)$$

with

$$\alpha := \frac{2048}{3} \kappa \gamma^2 (\gamma l_P^2)^{-5}. \quad (14)$$

Note that the Barbero-Immirzi parameter γ appears in α and also in the prefactor of the spectra (7) and (8). Therefore, quantitative results, which are also discussed later in the paper, will depend on the value of this parameter. Technically, γ arises as a quantization ambiguity which has to be fixed by observations or by comparing the results of explicit calculations with those obtained by other means. This has been done using the expected Bekenstein-Hawking result for the entropy of a black hole which yields the value $\gamma = \log 2/\pi \sqrt{3} \approx 0.13$ independently of the black hole parameters [18,19]. In the flat isotropic model studied here, γ can be understood physically as a parameter controlling the continuum limit [7], just as \hbar controls the classical limit. In the full theory, a similar role of γ in this context is not clear.

Equation (13) is a difference equation of order 8 for the wave function $s_n(\phi)$ in the internal time n . *A priori*, there could be a problem at zero volume since some of the coefficients of the difference equation can vanish due to $V_{-1} = V_{-1/2} = V_0 = 0$. In fact, the coefficient of $s_0(\phi)$ —and only this one—always vanishes (note that, unlike in a classical equation, $\widehat{|a|^{-1}}$ annihilates the zero-volume state which represents the classical singularity). Thus, there is always a solution $s_n(\phi) = s_0(\phi) \delta_{n0}$ which is orthogonal to all other solutions and need not be taken further into account. The only free function then is $s_n(\phi)$ for $n=4$, from which one can compute s_8 , and so on, yielding all coefficients $s_{4m}(\phi)$ as functions of $s_4(\phi)$. The intermediate values $s_{4m+i}(\phi)$ for $i=1,2,3$ are essentially fixed by the principal series $s_{4m}(\phi)$ by requiring that the wave function does not vary strongly on small scales if n is large (i.e. that it is pre-classical [10]).

The simplest choice for the free function $s_4(\phi)$, besides a constant, is an eigenfunction of the matter Hamiltonian $\hat{H}_\phi(4)$ for $n=4$,

$$s_4(\phi) = \chi(\phi) := e^{i\omega\phi/\hbar} \quad (15)$$

where ω is the eigenvalue of \hat{p}_ϕ . (A spatially constant massless field on Minkowski space with a non-vanishing energy eigenvalue would not be possible, but here geometry acts as a potential.) Because $\chi(\phi)$ is an eigenfunction for all $\hat{H}_\phi(n)$, the ϕ dependence of all the s_{4m} is the same. This will simplify the analysis since we can compute the wave function from an ordinary difference equation rather than a difference-differential equation; the combination $s_n(\phi)e^{-i\omega\phi/\hbar}$ will be ϕ independent.

We do not intend to justify the initial condition (15) with any given ω by a physical argument; rather, we choose it to simplify the subsequent calculations while retaining qualitative aspects as to the behavior of the wave function $s_n(\phi)$

close to the classical singularity in the presence of matter. The advantage of an initial condition like Eq. (15) is that the gravitational and the matter degree of freedom separate such that the n behavior of the wave function is still given by an ordinary difference equation. If a more complicated function than Eq. (15) is required, it can always be constructed as a suitable superposition of our solutions with different ω .

III. SOLUTIONS OF THE HAMILTONIAN CONSTRAINT

Having made the above observations about s_0 and s_4 , we begin with inserting $n=4$ into Eq. (13) and obtain s_8 in terms of $s_4 = \chi(\phi)$,

$$s_8(\phi) = \frac{2(V_2 - V_1) - \alpha\omega^2(\sqrt{V_2} - \sqrt{V_1})^6}{V_4 - V_3} \chi(\phi)$$

and, in consequence, all

$$s_{4m}(\phi) = \frac{2(V_{2m-2} - V_{2m-3}) - \alpha\omega^2(\sqrt{V_{2m-2}} - \sqrt{V_{2m-3}})^6}{V_{2m} - V_{2m-1}} s_{4m-4}(\phi) - \frac{V_{2m-4} - V_{2m-5}}{V_{2m} - V_{2m-1}} s_{4m-8}(\phi) \quad \text{for } m \in \mathbb{N}. \quad (16)$$

For an explicit calculation of the coefficients s_{4m} it is convenient to introduce some shorthand notations. We define

$$D_n := V_n - V_{n-1} \quad \text{and} \quad W_n := (\sqrt{V_n} - \sqrt{V_{n-1}})^6,$$

then we split off the ϕ dependence by defining ϕ -independent coefficients r_m by $r_0=0$, $r_1=1$ and

$$s_{4m}(\phi) = \frac{r_m}{D_{2m}D_{2m-2}\dots D_4} \chi(\phi) \quad \text{for } m \geq 2.$$

Inserting this into Eq. (16) yields a recurrence relation for the r_m :

$$r_m = (2D_{2m-2} - \alpha\omega^2 W_{2m-2}) r_{m-1} - D_{2m-2} D_{2m-4} r_{m-2}. \quad (17)$$

An explicit solution can be found after calculating a few r_m , and confirmed by induction:

$$r_m = \sum_{k=0}^{m-1} (-\alpha\omega^2)^k \sum_{\{j_1, \dots, j_k\}} j_1(j_2 - j_1) \dots (j_k - j_{k-1}) \times (m - j_k) W_{2j_1} \dots W_{2j_k} D_{2j_{k+1}} \dots D_{2j_{m-1}}. \quad (18)$$

This formula has the following meaning: j_1, \dots, j_k are integers between 1 and $m-1$, according to the $\binom{m-1}{k}$ possibilities to choose k numbers out of $\{1, 2, \dots, m-1\}$, arranged in increasing order. The numbers j_{k+1}, \dots, j_{m-1} appearing as labels of D_n are given by the remaining values in $\{1, \dots, m-1\} \setminus \{j_1, \dots, j_k\}$ in an arbitrary ordering. The case $k=0$ is to be understood in the way that from the fac-

tors containing j there remains only the last one, $m - j_0$, with j_0 defined to be zero, so that this contribution is $m D_2 \dots D_{2(m-1)}$.

For the purpose of numerically calculating the coefficients in terms of a given initial one the recurrence relation (17) may be more convenient than the solution (18).

Inserting $n=0$ into Eq. (13) leads to $s_{-4}(\phi) = s_4(\phi)$. Further on, Eq. (13) is symmetric in the sense that the relations between s_{-4} , s_{-8} , s_{-12} , \dots are the same as the respective relations for s_4 , s_8 , s_{12} , \dots and so the series s_{4m} is symmetric in m . By the argument of pre-classicality [7] this symmetry applies to the remaining series s_{4m+i} as well. With the physical interpretation of n as an internal time we have obtained time symmetry of our wave function with respect to the classical singularity.

IV. CONTINUUM AND SEMICLASSICAL LIMIT

For large n , when V_n becomes very large in comparison with l_P^3 , the discreteness should only lead to small corrections, i.e. the discrete time evolution from n to $n+4$ should become well approximated by a continuous evolution. Under this assumption the difference equation should be approximated with high accuracy by a differential equation for a continuous wave function $\psi(p, \phi) = s_{n(p)}(\phi)$, where $n(p) = 6p/\gamma l_P^2$ can be derived from the volume eigenvalues (7). Usually, the original difference equation is of higher order than the resulting differential equation in the continuum approximation and thus has more independent solutions. However, most of these solutions will vary strongly if one goes from n to $n+1$, i.e. if the volume is changed by one Planck

cube. Such a solution cannot be expected to behave almost classically, not even at large volume. Only *pre-classical* [10] solutions which do not vary strongly at small scales if the volume is large can be allowed for a semiclassical analysis, and only those solutions can be recovered from the approximating differential equation. As discussed in [10], among the solutions of the difference equation there is always one which is slowly varying at small scales for large n and so justifies the assumption of pre-classical behavior.

A. Large volume behavior

To approximate Eq. (13) by a differential equation it is convenient first to make a slight change of variables. We define the new variable (working only with positive $n > 0$)

$$t_n(\phi) := (\gamma l_p^2)^{-1} (V_{n/2} - V_{n/2-1}) s_n(\phi) \quad (19)$$

which for large n is approximated by $t_n(\phi) \sim \frac{1}{2} \sqrt{p(n)} \psi(p(n), \phi) =: \tilde{\psi}(p(n), \phi)$. In terms of $t_n(\phi)$ the evolution equation becomes

$$\begin{aligned} & t_{n+4}(\phi) - 2t_n(\phi) + t_{n-4}(\phi) \\ &= \alpha \hbar^2 \frac{(\sqrt{V_{n/2}} - \sqrt{V_{n/2-1}})^6}{V_{n/2} - V_{n/2-1}} \frac{d^2}{d\phi^2} t_n(\phi). \end{aligned} \quad (20)$$

Furthermore, we need the asymptotic approximations

$$\begin{aligned} V_{n/2} - V_{n/2-1} &\sim 24^{-1/2} (\gamma l_p^2)^{3/2} n^{1/2} \\ &= \frac{1}{2} \gamma l_p^2 \sqrt{p(n)} (\sqrt{V_{n/2}} - \sqrt{V_{n/2-1}})^6 \\ &\sim \left(\frac{3}{128}\right)^{3/2} (\gamma l_p^2)^{9/2} n^{-3/2} \\ &= \left(\frac{1}{4}\right) \gamma l_p^2 p(n)^{-3/2}. \end{aligned}$$

For the differences operator on the left-hand side of Eq. (20) we obtain in the continuum limit $16\partial^2/\partial n^2 = \frac{4}{9}(\gamma l_p^2)^2 \partial^2/\partial p^2$, acting on the function $\tilde{\psi}(p, \phi)$, so the asymptotic equation becomes

$$\left[\frac{4l_p^4}{3\kappa\hbar^2} p^2 \frac{\partial^2}{\partial p^2} - \frac{\partial^2}{\partial \phi^2} \right] \tilde{\psi}(p, \phi) = 0. \quad (21)$$

Note that a standard quantization in geometrodynamics would have ordering ambiguities in the gravitational part of the Wheeler-DeWitt equation, whereas the derivation here leads to a unique ordering in loop quantum cosmology [4].

The variables in this partial differential equation can be separated by a product ansatz,

$$\tilde{\psi}(p, \phi) = N(p) \chi(\phi),$$

so that we obtain

$$\frac{4l_p^4}{3\kappa\hbar^2} p^2 \frac{N''}{N} = \frac{\chi''}{\chi} = -\omega^2/\hbar^2 = \text{const.}$$

We assume $\omega^2 > 0$, because the matter Hamiltonian is expected to have a positive spectrum. With this assumption the solution χ coincides with the function used for s_4 in Eq. (15), denoted by the same letter. The ordinary differential equation for $N(p)$ has the solutions $N(p) = p^\lambda$ with

$$\lambda = \frac{1}{2} \pm \sqrt{\frac{1}{4} - \frac{3}{4} \kappa \omega^2 l_p^{-4}}. \quad (22)$$

The asymptotic differential equation (21) applies also for t_{4m+i} for $i=1,2,3$, so, in order to have a smooth function for large n we assume the ϕ dependence of the remaining three free coefficients s_1 , s_2 and s_3 to be the same as that of s_4 , given by the function $\chi(\phi)$, endowed with constant factors which could be fitted by a numerical analysis.

The last result (22) deserves some discussion, because it provides a threshold for a qualitatively different behavior of the solution $N(p)$, according to the sign of the expression under the square root. If ω is smaller than a critical value, determined by

$$\omega_c^2 = \frac{1}{3} l_p^4 / \kappa = \frac{1}{3} \kappa \hbar^2, \quad (23)$$

the exponent λ is real and for ω going to zero one solution for $N(p)$ approaches p , the asymptotic function for the vacuum calculated in [4], the other one approaches a constant. For ω larger than ω_c

$$N(p) = p^{1/2} p^{\pm i\Omega} = p^{1/2} e^{\pm i\Omega \log p} \quad (24)$$

with

$$\Omega = \frac{1}{2} \sqrt{3\kappa\omega^2 l_p^{-4} - 1} = \frac{1}{2} \hbar^{-1} \sqrt{3\omega^2/\kappa - \hbar^2}. \quad (25)$$

Reconstructing $\psi(p, \phi)$ from $\tilde{\psi}(p, \phi)$ we finally obtain

$$\psi(p, \phi) = 2e^{\pm i\Omega \log p} e^{i\omega\phi/\hbar}. \quad (26)$$

Formally this solution is a quantum mechanical wave function of a particle moving from small values of p to larger ones with decreasing speed, whereas solutions with real powers of p , coming from undercritical values of ω , are lacking such a dynamical interpretation. An example of an oscillating solution can be seen in Fig. 1 for $\omega^2 = 500\omega_c^2$, a non-oscillating one with $\omega^2 = \frac{1}{2}\omega_c^2$ in Fig. 2.

Note that the presence of a critical frequency ω_c depends on the ordering of the Wheeler-DeWitt equation; choosing, e.g., the ordering $p\partial/\partial p(p\partial/\partial p)$ instead of $p^2\partial^2/\partial p^2$ would give oscillating solutions for all non-zero ω . Therefore, standard quantum cosmology cannot imply such a behavior reliably. Loop quantum cosmology, on the other hand, has a distinguished ordering and thus predicts the existence of a critical frequency for the system studied here.

Before interpreting the physical significance of ω_c we note that the possibility of a non-oscillating wave function

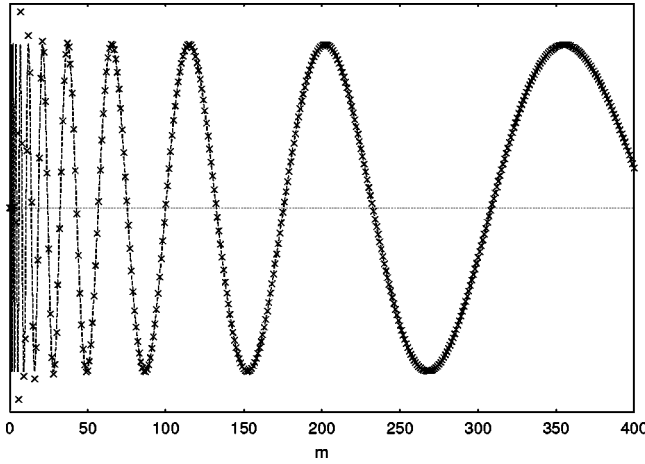


FIG. 1. The ϕ -independent part $s_{4m}(\phi)e^{-i\omega\phi/\hbar}$ of the discrete wave function (\times) compared to a continuous solution to the Wheeler-DeWitt equation (dashed line) for $\omega^2 = 500\omega_c^2$. Strong deviations occur only at very small $n = 4m$ (see Fig. 4) and will be discussed later.

for $\omega^2 < \omega_c^2$ is not in contradiction with semiclassical behavior at large volume. The standard semiclassical analysis requires oscillating (WKB) solutions which in our case can be derived from Eq. (3) after replacing c with $\frac{1}{3}\gamma\kappa\partial S/\partial p$ and are given by $N_{WKB}(p) = \exp(iS/\hbar) = \exp(i\Omega_{WKB}\log p)$ with $\Omega_{WKB} = \frac{1}{2}\sqrt{3\kappa\omega/l_P^2}$. For $\omega^2 \gg \omega_c^2$ the frequency Ω in fact reduces to Ω_{WKB} . The non-oscillating solutions for $\omega^2 < \omega_c^2$ cannot be interpreted in this way, but this should not be expected since in the classical limit $\omega_c = \frac{1}{3}\kappa\hbar^2$ vanishes and so any non-zero frequency will be larger than the critical one.

B. A critical energy

We have seen that loop quantum cosmology predicts the presence of a critical frequency for a dynamical evolution in the particular model studied here. While this prediction is reliable (in contrast to standard quantum cosmology where it may or may not exist, depending on the factor ordering of the constraint), we will see that the precise value depends on quantization ambiguities of a different kind.

For an interpretation of ω_c we first compute the associated ($1/a$ -dependent) eigenvalues of the matter Hamiltonian,

$$E(a) = \frac{1}{2}|a|^{-3}\omega^2. \quad (27)$$

In standard quantum cosmology, this expression is unbounded from above and does not have a distinguished value which would be suitable for an interpretation. In loop quantum cosmology, on the other hand, we do have—for a given ω —an upper bound for E which can serve as a natural value for an interpretation. Taking for $1/|a|$ the maximal eigenvalue of the inverse scale factor operator, occurring at $n = 2$, we get a relation between the maximal field energy concentrated in $V_{1/2} = \frac{1}{6}(\gamma l_P^2)^{3/2}$ and ω^2 :

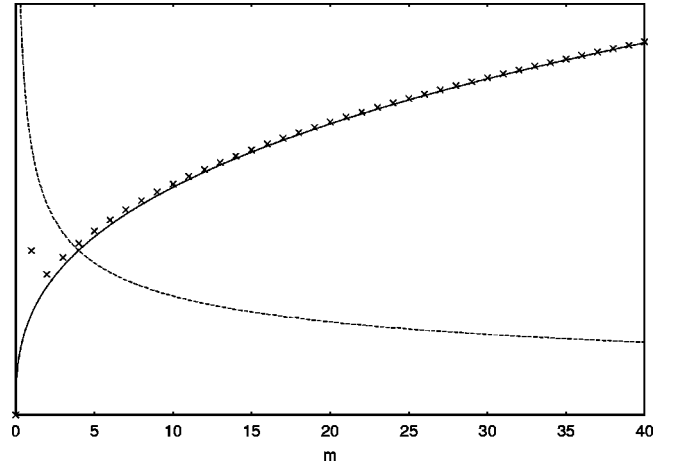


FIG. 2. A subcritical ($\omega^2 = \frac{1}{2}\omega_c^2$) wave function $s_{4m}(\phi)e^{-i\omega\phi/\hbar}$ compared with the continuous DeWitt wave function (solid line) and a continuous wave function which does not satisfy DeWitt's initial condition (dashed line; any such solution diverges at $a = 0$).

$$E_{\max} = \frac{2^{11}}{3^3(\gamma l_P^2)^{3/2}}\omega^2.$$

By inserting ω^2 into Eq. (25) the distinction between oscillating and non-oscillating behavior can be expressed in terms of this initial energy,

$$\Omega = \frac{9\sqrt{\pi}}{32}\gamma^{3/4}\sqrt{\frac{E_{\max}}{E_P} - \frac{256}{81\pi}}\gamma^{-3/2}, \quad (28)$$

with E_P denoting the Planck energy $8\pi\hbar/l_P = l_P/G$. This expresses Ω in terms of the ratio E_{\max}/E_P , whose critical value $(256/81\pi)\gamma^{-3/2} \approx 1.006$ is close to one for γ equal to one, but has the larger value ≈ 21.5 for the value $\gamma = \log 2/\pi\sqrt{3} \approx 0.13$ which has been computed by comparing the black hole entropy resulting from a counting within quantum geometry with the semiclassical Bekenstein-Hawking result [18,19]. Only if E_{\max}/E_P is larger than the critical value can a dynamical evolution of the classical Friedmann model set in.

This observation implies that we need a maximal energy in a Planck volume which *exceeds* the Planck energy, being apparently in conflict with the heuristic but widespread expectation that there can be at most an energy amount of E_P in a Planck volume. (Often, the holographic principle [20] is used to arrive at this conclusion. In the present context, there is no direct contradiction of results obtained within the formalism used here.) Usually, inflation is invoked to explain how the huge amount of energy in the present universe can have originated from a Planck scale universe. Here we can see that the relation between the maximal energy and inflation is even more intimate in loop quantum cosmology: One can reduce the critical value for E_{\max}/E_P by using a different

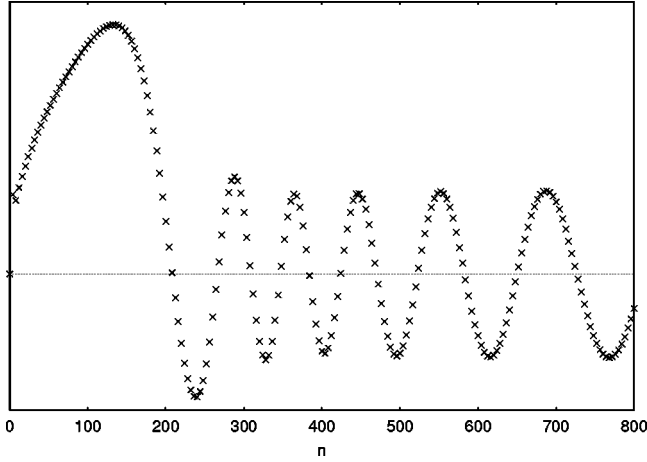


FIG. 3. A wave function with an extended inflationary phase ($j=200$) and standard behavior at large volume for $n > 2j = 400$ ($\omega^2 = 500\omega_c^2$).

quantization for the inverse scale factor instead of Eq. (8) parametrized by an ambiguity parameter j (a non-zero half-integer, see [17]) such that

$$|\widehat{a|_j^{-1}}|n\rangle = 144[j(j+1)(2j+1)]^{-2}(\gamma l_P^2)^{-2} \times \left(\sum_{k=-j}^j k \sqrt{V_{(|n+2k|-1)/2}} \right)^2. \quad (29)$$

As derived in [17], the maximal value of $|a|_j^{-3}$ is then attained if $n=2j$ and approximately given by V_j^{-1} (the approximation gets better for large j). This gives a maximal energy

$$E_{\max,j} \sim \frac{1}{2} \omega^2 V_j^{-1} \sim \frac{1}{2} \omega^2 (\gamma l_P^2)^{-3/2} (3/j)^{3/2}$$

and

$$\Omega \sim \sqrt{4\pi} 3^{-1/4} (\gamma j)^{3/4} \sqrt{\frac{E_{\max,j}}{E_P} - \frac{\sqrt{3}}{16\pi(\gamma j)^{3/2}}}.$$

The critical value $(\sqrt{3}/16\pi)(\gamma j)^{-3/2} \approx 0.74j^{-3/2}$ for E_{\max}/E_P is then suppressed by $j^{-3/2}$ and much smaller than one for large j (note that this critical value for $j = \frac{1}{2}$ does not coincide with the one obtained above because the approximation for the maximum of Eq. (29) is bad for very small j). Moreover, the maximal energy is not obtained in the initial Planck volume but in a volume of size $V_j \sim (\frac{1}{3}j\sqrt{\gamma}l_P)^3$. As observed in [21], using a quantization with a large value of j also leads to a prolonged phase of inflation in the very early universe, displaying the relation between a maximal energy below the Planck energy and inflation.

A large value of j modifies the small volume behavior of the wave function considerably (Fig. 3). Its oscillation length and amplitude first decrease with increasing volume, which is characteristic of an accelerating universe. When the maxi-

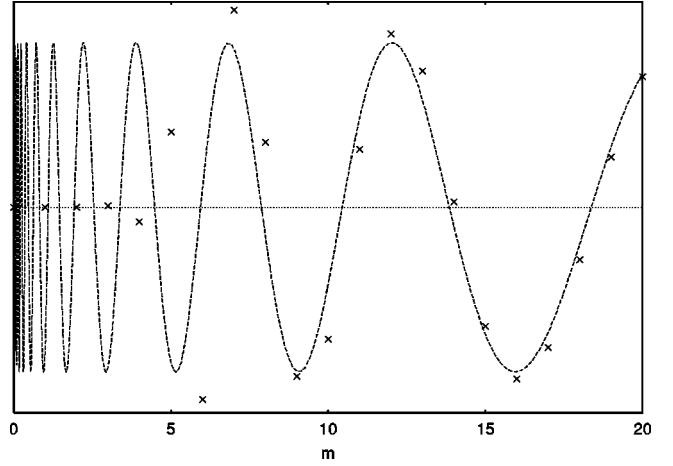


FIG. 4. The small- m behavior of the ϕ -independent part $s_{4m}(\phi)e^{-i\omega\phi/\hbar}$ of the discrete wave function (\times) compared to a continuous solution to the Wheeler-DeWitt equation (dashed line) for $\omega^2 = 500\omega_c^2$. Whereas the continuous solution displays an infinite number of oscillations, the discrete solution decreases toward zero once the oscillation length is comparable to the Planck scale.

mal value for $|a|_j^{-3}$ is reached, standard behavior (26) sets in with increasing oscillation length toward larger volume.

V. COMPARISON WITH CONTINUUM INITIAL CONDITIONS

In loop quantum cosmology the initial conditions for the gravitational part of the wave function are derived from the evolution equation and thus fixed [10]. While s_0 , the value of the wave function at the classical singularity, drops out of the evolution equation and so remains unspecified, the lowest values of n show that the wave function approaches the value zero for small n (see Figs. 1 and 4). Interpreted as an initial value, this is reminiscent of DeWitt's proposal that the continuum wave function $\psi(a)$ should vanish for $a=0$ [1]. It is well known that DeWitt's initial condition can be satisfied non-trivially only in special systems (e.g., for quantum de Sitter space); generically it would imply that the wave function vanishes identically.

An example for a system where DeWitt's condition does not work in general is the one discussed in the present paper: Eq. (26) is a continuous wave function which does not have a well-defined limit for $a \rightarrow 0$ if $\omega^2 > \omega_c^2$ because it oscillates with constant amplitude and diverging frequency close to the classical singularity (for $\omega^2 < \omega_c^2$ DeWitt's initial condition can be defined and coincides with the result of the dynamical initial condition; see Fig. 2). Another example is [22] where a wave function of the same kind as Eq. (26) was obtained for stiff matter and rejected because it does not satisfy a DeWitt boundary condition in the sense that either the function or its derivative should be equal to zero at the classical singularity. The same is true for the continuum approximation of our wave function, but in this case the problem is cured by discreteness near the singularity.

The oscillations are suppressed once their oscillation length becomes smaller than the Planck length, and conse-

quently their amplitude approaches zero. (If there is prolonged inflation with a large value of j , as discussed above, the oscillation length may never reach the Planck length where this mechanism would be necessary. For a fixed j , however, a regime with small oscillation length will always be present if ω is large enough.) This can be seen by following the analysis of [10]: If we define

$$P(n) := \frac{1}{3} \kappa \gamma l_p^2 H_\phi(n) (V_{n/2} - V_{n/2-1})^{-1}$$

which at large volume is approximately $P \sim \frac{2}{3} \kappa H_\phi / a$, the discrete evolution equation (20) is

$$t_{n+4} - [2 - \gamma^2 P(n)] t_n + t_{n-4} = 0.$$

In the neighborhood of a fixed n we can assume that $P(n)$ is a constant and solve the difference equation with an ansatz $t_n = e^{in\theta}$ which leads to

$$e^{4i\theta} - (2 - \gamma^2 P) + e^{-4i\theta} = 2 \cos 4\theta - 2 + \gamma^2 P = 0.$$

If P is small, the solution $\theta = \frac{1}{4} \arccos(1 - \gamma^2 P/2)$ is real and small, implying an oscillating wave function $t_n = e^{in\theta}$ with long oscillation length $2\pi/\theta \approx \pi/\gamma\sqrt{P}$ as observed at large volume. [This conclusion is only valid if the resulting oscillation length is smaller than the length scale on which $P(n)$ changes substantially. In particular, it does not apply to subcritical solutions for which the predicted oscillation length would be too large.] As P becomes larger, which will happen for decreasing a , θ will first increase up to $\theta_{\max} = \pi/4$ (for $P = 2\gamma^{-2}$) and then become imaginary. The result is that the wave function will first oscillate more and more rapidly, as expected from the continuum approximation, but then enter a branch with exponential behavior which does not appear in the continuum formulation. Of the two independent solutions—exponentially increasing or decreasing—only the decreasing one is allowed by the dynamical initial conditions (Fig. 4). This is the mechanism, essentially relying on the discreteness, which allows us to generalize DeWitt's initial condition to systems where the continuum version does not work. (Note that a similar behavior with exponential solutions can occur at large volume in the presence of a positive cosmological constant. In such a case, it would be caused by large volume rather than large curvature and therefore signals an infrared problem. In the small volume regime, however, a modified behavior is perfectly admissible and welcome since the classical description is expected to break down if curvatures become large.)

The diverging oscillation number close to $a=0$ renders inapplicable not only DeWitt's proposal but any condition which requires properties of the continuous wave function at $a=0$, which includes the “no-boundary” and the “tunneling” proposals. (Usually, this problem is avoided by setting $\omega=0$ or an analogous condition by hand, see e.g. [23]. Note that this is a very strong assumption since even a tiny ω would eventually yield a large kinetic term due to the inverse volume.) As already discussed, of the proposed initial condi-

tions only the discrete formulation of loop quantum cosmology can deal with the problem of wild oscillations close to the classical singularity.

VI. CONCLUSIONS

In this paper we considered a free massless scalar field coupled to loop quantum cosmology as a model for implications of the kinetic term in a matter Hamiltonian. This term diverges classically at zero volume and is also problematic in standard quantum cosmology where it leads to infinitely many oscillations of the wave function close to the classical singularity. It is caused by the inverse volume in the kinetic term and is not sensitive to the special form of matter or its quantization. Therefore, we restricted our attention to the free massless scalar field quantized in a standard way as usual in the Wheeler-DeWitt approach. A possible mass or potential term, which is proportional to the volume, would not change the qualitative behavior at small enough volume where it would be suppressed. Also higher spin fields or different quantization techniques applied to the matter field, e.g. inspired by methods for full quantum geometry [15], would not be significant as far as the present paper is concerned. We also note that we simplified the analysis by using only the Euclidean part of the gravitational constraint multiplied with γ^{-2} instead of the full Lorentzian constraint in Eq. (9). In the flat case, both expressions agree classically, and at the quantum level the more complicated Lorentzian constraint does not lead to significant changes of the qualitative behavior.

The quantization of the gravitational degrees of freedom, on the other hand, is important since it affects the form of the inverse volume in a quantization of the kinetic term. While standard quantum cosmology treats the inverse volume as a multiplication operator which does not cure its divergence, loop quantum cosmology leads to a quantization with significant changes at small scales where the discreteness of the volume is important and its inverse does not diverge. This has already been seen to imply the absence of cosmological singularities [9], dynamical initial conditions for the wave function of a universe [10], and a new origin of inflation [21]. The main result of the present paper is that the discreteness at small scales also leads to a cure of pathologies of the wave function in a standard quantization, like the infinite number of oscillations caused by a kinetic matter term.

Also the issue of initial conditions is further elucidated by this analysis. In [10] it has been shown that loop quantum cosmology predicts dynamical initial conditions for the wave function of a universe which can be derived from the evolution equation and need not be imposed by hand. In this derivation the structure of the cured classical singularity plays an important role. In their effect on the wave function the dynamical initial conditions resemble most closely DeWitt's initial condition that the wave function should vanish at the classical singularity. The drawback of DeWitt's approach, namely that this initial condition cannot be fulfilled non-trivially for most systems of physical interest, has been seen to be eliminated by effects of the discreteness of loop quantum cosmology. Therefore, *the dynamical initial conditions*

of loop quantum cosmology present a meaningful generalization of DeWitt's initial conditions.

We also emphasize that loop quantum cosmology leads to more reliable results than standard quantum cosmology because some quantization ambiguities like the factor ordering of the gravitational part of the constraint are fixed (while it shares the feature of being a minisuperspace quantization which freezes infinitely many degrees of freedom). Nevertheless there are ambiguities of a different kind which can affect physical consequences and therefore in principle lead to observable effects. This has played a role in the discussion of a critical matter energy necessary for an oscillating wave function in the particular model studied here. Its value de-

pends on the quantization ambiguities, but its presence can be concluded from loop quantum cosmology, unlike standard quantum cosmology where it may or may not occur depending on the ordering.

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