

Isotropic Loop Quantum Cosmology

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Abstract

Isotropic models in loop quantum cosmology allow explicit calculations, thanks largely to a completely known volume spectrum, which is exploited in order to write down the evolution equation in a discrete internal time. Because of genuinely quantum geometrical effects the classical singularity is absent in those models in the sense that the evolution does not break down there, contrary to the classical situation where space-time is inextendible. This effect is generic and does not depend on matter violating energy conditions, but it does depend on the factor ordering of the Hamiltonian constraint. Furthermore, it is shown that loop quantum cosmology reproduces standard quantum cosmology and hence (e.g., via WKB approximation) to classical behavior in the large volume regime where the discreteness of space is insignificant. Finally, an explicit solution to the Euclidean vacuum constraint is discussed which is the unique solution with semiclassical behavior representing quantum Euclidean space.

1 Introduction

General relativity is a very successful theory for the gravitational field which is well tested in the weak field regime. However, it also implies the well-known singularity theorems [1] according to which singularities and therefore a breakdown of this theory are unavoidable provided that matter behaves in a classically reasonable manner (i.e., fulfills energy conditions). In fact, observations of the cosmic microwave background demonstrate that the universe was in a very dense state a long time ago, which classically can be understood only in models which have an initial singularity.

However, if the universe is small and the gravitational field strong, the classical description is supposed to break down and to be replaced by a quantum theory of gravity. In early attempts it was proposed that the singularity could be avoided by coupling classical or quantum matter fields which violate the strong energy condition and thereby evade the

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singularity theorems [2, 3, 4, 5]. Another approach modifies the field equations by adding higher curvature terms interpreted as the leading order corrections of quantum gravity [6, 7, 8]. However, the first approach uses matter effects rather than those of quantum gravity, and in the second, more and more corrections are needed the closer one comes to the classical singularity. Furthermore, the procedure of truncating the series of perturbative corrections (involving higher derivatives), and treating all solutions to the resulting equations of high order on the same footing as those of the lowest order ones, is inconsistent [9]. Eventually one still needs a full non-perturbative quantum theory of gravity in order to understand the fate of the singularity.

Lacking a full quantization of general relativity, an early approach to quantum cosmology was to perform a symmetry reduction to homogeneous or isotropic models with a finite number of degrees of freedom and to quantize afterwards [10, 11]; this will be called “standard quantum cosmology” in the following. But in general, those models do not avoid the classical singularity (even the meaning of this phrase is not clearly understood: an early idea was to impose the condition that the wave function $\psi(a)$ vanishes at the singularity $a = 0$ [10], but this is insufficient with a continuous spectrum of the scale factor a [12] which is always the case in standard quantum cosmology), and more severely quantum mechanical methods are used for the quantization which are not believed to be applicable to a full quantization of general relativity. Therefore, it is not clear to what extent the results are relevant for quantum gravity.

In the meantime, a candidate for quantum gravity has emerged which is now called quantum geometry [13, 14]. A key success of this approach is the derivation of a discrete structure of space which is implied by the discreteness of spectra of geometric operators like area and volume [15, 16, 17]. It also leads to a new approach to quantum cosmology [18]: By reducing this kinematical quantum field theory to homogeneous or isotropic states using the general framework for such a symmetry reduction at the quantum level [19] one arrives at loop quantum cosmology [20]. Due to this derivation loop quantum cosmology is very different from standard quantum cosmology; e.g., the volume is discrete [21] which is inherited from quantum geometry. As a consequence the Hamiltonian constraint, which governs the dynamics, of those models [22] can be written as a difference equation rather than the differential, Schrödinger- or Klein-Gordon-like evolution equation of standard quantum cosmology; thus, also time is discrete [23]. One may expect that the discrete structure of space-time, which is most important at small volume, will have dramatic consequences for the appearance of a singularity¹. As a loose analogy one may look at the hydrogen atom: classically it has a continuous family of orbits leading to its instability, which is quantum mechanically cured by allowing only a discrete set of states. Of course, one also has to determine radiation loss or transition rates to judge stability, i.e. one has to take into account the fully dynamical situation.

In fact techniques developed for a quantization of the full theory [24] can be used to show in isotropic models that the inverse scale factor, whose divergence signals the singularity in the classical model, can be quantized to a bounded operator with finite eigenvalues even in

¹The author is grateful to A. Ashtekar for suggesting this idea and for discussions about this issue.

states which are annihilated by the volume operator [25]. This is already a first indication that close to the classical singularity the system is at least better behaved in a quantum theory of geometry, which is to be confirmed by studying the dynamics of these models as governed by the Hamiltonian constraint equation. The results of this analysis have been communicated in [26] and are described in detail in the present paper: whereas the classical singularity presents a boundary of space-time which can be reached in finite proper time but beyond which an extension of space-time is impossible, the quantum evolution equation does not break down at the classical singularity provided only that we choose the appropriate factor ordering of the constraint. The conclusion is, however, independent of the particular matter coupled to the model, and so does not rely on special forms of matter violating energy conditions. We will describe these conclusions in detail in Section 4 after reviewing the formalism of isotropic loop quantum cosmology (Section 2) and computing the action of the Hamiltonian constraint for spatially flat models (Section 3; the constraint for positively curved models can be found in App. B). After discussing the fate of the singularity in Section 4.2 we will see in Section 4.3 that we simultaneously have the correct semiclassical behavior at large volume, and present in Section 5.1 an explicit solution to the vacuum Euclidean constraint which gives quantum Euclidean space. A comparison with other approaches and ideas put forward to avoid or resolve the singularity can be found in Section 6 before our conclusions where we will also discuss in which sense, compared to the classical singularity theorems, the singularity is absent in loop quantum cosmology.

2 Isotropic Loop Quantum Cosmology

A calculus for isotropic models of loop quantum cosmology can be derived from that of quantum geometry along the lines of the general framework for a symmetry reduction of diffeomorphism invariant quantum field theories [19]. This allows us to perform the symmetry reduction at the quantum level by selecting symmetric states. In the connection representation, those states are by definition only supported on connections being invariant with respect to the given action of the symmetry group. They can be embedded in the full kinematical Hilbert space as distributional states.

Specializing this framework to isotropy [20] leads to isotropic states supported on isotropic connections of the form $A_a^i = \phi_I^i \omega_a^I = c \Lambda_I^i \omega_a^I$. Here, the internal $SU(2)$ -dreibein $\Lambda_I = \Lambda_I^i \tau_i$ is purely gauge ($\tau_j = -\frac{i}{2} \sigma_j$ are generators of $SU(2)$ with the Pauli matrices σ_j) and ω^I are left-invariant one-forms on the “translational” part N (isomorphic to \mathbb{R}^3 for the spatially flat model or $SU(2)$ for the spatially positively curved model) of the symmetry group $S \cong N \rtimes SO(3)$ acting on the space manifold Σ . Orthonormality relations for the internal dreibein are

$$\Lambda_I^i \Lambda_i^J = \delta_I^J \quad \text{and} \quad \epsilon_{ijk} \Lambda_I^i \Lambda_J^j \Lambda_K^k = \epsilon_{IJK}. \quad (1)$$

For homogeneous models, the nine parameters ϕ_I^i are arbitrary, and for isotropic models c is the only gauge-invariant parameter. A co-triad can be expressed as $e_a^i = a_I^i \omega_a^I = a \Lambda_I^i \omega_a^I$ with the scale factor $|a|$ (in a triad formulation it is possible to use a variable a

which can take both signs even though the two corresponding sectors are disconnected in a metric formulation). Using left-invariant vector fields X_I fulfilling $\omega^I(X_J) = \delta_J^I$, momenta canonically conjugate to A_a^i are densitized triads of the form $E_i^a = p_i^I X_I^a = p \Lambda_i^I X_I^a$ where $p = \text{sgn}(a)a^2$. Besides gauge degrees of freedom, there are only the two canonically conjugate variables c and p which have the physical meaning of curvature and square of radius, and are coordinates of a phase space with symplectic structure

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

($\kappa = 8\pi G$ is the gravitational constant and γ the Barbero–Immirzi parameter; see [25] for an explanation of the correct factor $\frac{1}{3}$ which is missing in [21]).

Any gauge invariant isotropic state, being supported only on isotropic connections, can be expressed as a function of c . An orthonormal basis of such functions is given by the usual characters on $SU(2)$

$$\chi_j = \frac{\sin(j + \frac{1}{2})c}{\sin \frac{1}{2}c} \quad , \quad j \in \frac{1}{2}\mathbb{N}_0 \quad (3)$$

together with $\zeta_{-\frac{1}{2}} = (\sqrt{2} \sin \frac{1}{2}c)^{-1}$ and

$$\zeta_j = \frac{\cos(j + \frac{1}{2})c}{\sin \frac{1}{2}c} \quad , \quad j \in \frac{1}{2}\mathbb{N}_0. \quad (4)$$

Gauge non-invariant functions are given by $\Lambda_I^i \chi_j$ and $\Lambda_I^i \zeta_j$ where Λ_I^i is the internal dreibein providing pure gauge degrees of freedom.

The states χ_j, ζ_j are also eigenstates of the volume operator [21] with eigenvalues

$$V_j = (\gamma l_P^2)^{\frac{3}{2}} \sqrt{\frac{1}{27}j(j + \frac{1}{2})(j + 1)}. \quad (5)$$

Because j can take the value $-\frac{1}{2}$ as label of ζ_j the eigenvalue zero is threefold degenerate, whereas all other eigenvalues are positive and twice degenerate. An extension of the volume operator to gauge non-invariant states is done by using the relation $[\Lambda_I^i, \hat{V}] = 0$ which follows from gauge invariance of the volume [25].

Because the basic multiplication operator is the point holonomy $h_I := \exp(c\Lambda_I^i \tau_i) = \cos(\frac{1}{2}c) + 2\sin(\frac{1}{2}c)\Lambda_I^i \tau_i$ we also need the action of $\cos \frac{1}{2}c$ and $\sin \frac{1}{2}c$. This can be obtained in the connection representation (3), (4) by using trigonometric relations, but it is easier first to introduce a new orthonormal basis of the states

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

which are decomposed in the previous states by

$$|n\rangle = 2^{-\frac{1}{2}} \left(\zeta_{\frac{1}{2}(|n|-1)} + i \text{sgn}(n) \chi_{\frac{1}{2}(|n|-1)} \right)$$

for $n \neq 0$ and $|0\rangle = \zeta_{-\frac{1}{2}}$. The label n , which will appear as internal time label below, is the eigenvalue of the dreibein operator [21]

$$\hat{p} = \widehat{\Lambda_3^i E_i^3} = -\frac{1}{3}i\gamma l_P^2 \left(\frac{d}{dc} + \frac{1}{2} \cot \frac{1}{2}c \right).$$

On these states the action of $\cos \frac{1}{2}c$ and $\sin \frac{1}{2}c$ is

$$\cos(\tfrac{1}{2}c)|n\rangle = \tfrac{1}{2} \left(\exp(\tfrac{1}{2}ic) + \exp(-\tfrac{1}{2}ic) \right) \frac{\exp(\tfrac{1}{2}inc)}{\sqrt{2} \sin(\tfrac{1}{2}c)} = \tfrac{1}{2}(|n+1\rangle + |n-1\rangle) \quad (7)$$

$$\sin(\tfrac{1}{2}c)|n\rangle = -\tfrac{1}{2}i \left(\exp(\tfrac{1}{2}ic) - \exp(-\tfrac{1}{2}ic) \right) \frac{\exp(\tfrac{1}{2}inc)}{\sqrt{2} \sin(\tfrac{1}{2}c)} = -\tfrac{1}{2}i(|n+1\rangle - |n-1\rangle) \quad (8)$$

and that of the volume operator is

$$\hat{V}|n\rangle = V_{\frac{1}{2}(|n|-1)}|n\rangle = (\tfrac{1}{6}\gamma l_P^2)^{\frac{3}{2}} \sqrt{(|n|-1)|n|(|n|+1)}|n\rangle. \quad (9)$$

Together with the volume operator the trigonometric operators establish a complete calculus for isotropic cosmological models and more complicated operators can be constructed out of them. As a first application the expression $m_{IJ} := q_{IJ}/\sqrt{\det q} = |a|^{-1}\delta_{IJ}$ of the inverse scale factor has been quantized [25] using techniques developed in quantum geometry in order to quantize co-triad components, which are not fundamental variables [24]. The same method, which also leads to densely defined quantizations of matter Hamiltonians [27], results in a *bounded* operator quantizing the inverse scale factor

$$\begin{aligned} \hat{m}_{IJ} = & 16(\gamma l_P^2)^{-2} \left(4 \left(\sqrt{\hat{V}} - \cos(\tfrac{1}{2}c) \sqrt{\hat{V}} \cos(\tfrac{1}{2}c) - \sin(\tfrac{1}{2}c) \sqrt{\hat{V}} \sin(\tfrac{1}{2}c) \right)^2 \right. \\ & \left. - \delta_{IJ} \left(\sin(\tfrac{1}{2}c) \sqrt{\hat{V}} \cos(\tfrac{1}{2}c) - \cos(\tfrac{1}{2}c) \sqrt{\hat{V}} \sin(\tfrac{1}{2}c) \right)^2 \right) \end{aligned} \quad (10)$$

which has been studied in detail in [25]. We will later need the action

$$\begin{aligned} \left(\sin(\tfrac{1}{2}c) \hat{V} \cos(\tfrac{1}{2}c) - \cos(\tfrac{1}{2}c) \hat{V} \sin(\tfrac{1}{2}c) \right) |n\rangle &= \tfrac{1}{2}i \left(V_{\frac{1}{2}(|n+1|-1)} - V_{\frac{1}{2}(|n-1|-1)} \right) |n\rangle \\ &= \tfrac{1}{2}i \operatorname{sgn}(n) \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) |n\rangle \end{aligned} \quad (11)$$

(for $n = 0$ the value of V_{-1} is understood to be zero). Important for the results of the present article is that the state $|0\rangle = \zeta_{-\frac{1}{2}}$ is annihilated by both the volume operator and the inverse scale factor. This would, of course, be impossible in a classical theory and is a purely quantum geometrical effect. (Since the singularity $a = 0$ is not part of the classical phase space, one has to extend the inverse scale factor appropriately which is done here formally by $\operatorname{sgn}(a)^2/a$ [25].) Our later considerations crucially depend on the fact that all metrical operators, and therefore all matter Hamiltonians which in some way always contain metric components, annihilate the state $|0\rangle$.

3 Hamiltonian Constraint for Isotropic Models

For homogeneous models [20] the Euclidean part (which is the full constraint in Euclidean signature if $\gamma = 1$) of the Hamiltonian constraint is given by (the lapse function is irrelevant for cosmological models and set to be one)

$$\begin{aligned} H_{\text{hom}}^{(\text{E})} &= -\kappa^{-1} \det(a_I^i)^{-1} \epsilon_{ijk} F_{IJ}^i E_j^I E_k^J \\ &= \kappa^{-1} \det(a_I^i)^{-1} (\epsilon_{ijk} c_{IJ}^K \phi_K^i p_j^I p_k^J - \phi_I^j \phi_J^k p_j^I p_k^J + \phi_I^k \phi_J^j p_j^I p_k^J) \end{aligned} \quad (12)$$

(F_{IJ}^i are the curvature components of the connection A_I^i and c_{IJ}^K are the structure constants of the symmetry group). Here, we had to choose a relative sign for the constraint in the two different orientations of the triad. Classically, both orientations are disconnected because one has to require a non-degenerate triad. However, this is no longer necessary in a quantum theory, and we will in fact see that an evolution through degenerate metrics is possible. Therefore we have to choose the relative sign which we did by using the determinant of the co-triad instead of the metric, which would always be positive. The quantization techniques of [24] directly apply only to the convention in (12). We will see that one can transform between the two choices after quantization, however not unambiguously due to special features at the classical singularity; see the remarks following (22).

3.1 The Classical Constraint

In the present context of isotropic models we are interested only in special homogeneous models which can be further reduced to isotropy. These are the two Bianchi class A models given by the structure constants $c_{IJ}^K = 0$ (Bianchi type I) which lead to the isotropic spatially flat model or $c_{IJ}^K = \epsilon_{IJ}^K$ (Bianchi type IX) leading to the isotropic model with positive spatial curvature. The third isotropic model, which has negative spatial curvature, can only be derived from a class B model and so is not accessible in the present framework. Inserting isotropic connection and triad components into (12) yields

$$H^{(\text{E})} = 6\kappa^{-1} a^{-3} (2\Gamma - c) c p^2 = 6\kappa^{-1} (2\Gamma - c) c \operatorname{sgn}(p) \sqrt{|p|} \quad (13)$$

where $\Gamma = 0$ for the flat model and $\Gamma = \frac{1}{2}$ for the positively curved model.

The parameter Γ also determines the spin connection compatible with a given triad, which is given by [28]

$$\Gamma_a^i = -\frac{1}{2} \epsilon^{ijk} e_j^b (2\partial_{[a} e_{b]}^k + e_k^c e_a^l \partial_c e_b^l).$$

For homogeneous triads $e_i^a = a_i^I X_I^a$ and inverse co-triads $e_a^i = a_I^i \omega_a^I$ this specializes to

$$\Gamma_a^i = -\epsilon^{ijk} a_j^J X_J^b (a_K^k \partial_{[a} \omega_{b]}^K + \frac{1}{2} a_k^K a_I^l a_L^l X_K^c \omega_a^I \partial_{[c} \omega_{b]}^L)$$

which using the Maurer–Cartan relations $\partial_{[a} \omega_{b]}^I = -\frac{1}{2} c_{JK}^I \omega_{[a}^J \omega_{b]}^K$ yields

$$\Gamma_a^i = \frac{1}{2} \epsilon^{ijk} (c_{IJ}^K a_j^J a_K^k + \frac{1}{2} c_{KJ}^L a_j^J a_k^K a_I^l a_L^l) \omega_a^I =: \Gamma_I^i \omega_a^I.$$

In isotropic models the co-triad has the special form $a_I^i = a\Lambda_I^i$ which implies $a_i^I = a^{-1}\Lambda_i^I$ and leads to

$$\Gamma_I^i = \frac{1}{2}c_{IJ}^K\epsilon_{KL}^J\Lambda_L^i + \frac{1}{4}c_{KJ}^L\epsilon^{JKM}\Lambda_M^i\delta_{IL}$$

using the orthonormality relations (1) for the internal dreibein Λ_I^i . Now we use that for Bianchi class A models the structure constants have the form $c_{IJ}^K = \epsilon_{IJL}n^{LK}$ where $n^{LK} = n^{(K)}\delta^{LK}$ is a diagonal matrix with $n^I = 0$ for Bianchi I and $n^I = 1$ for Bianchi IX. With these structure constants we finally arrive at

$$\Gamma_I^i = \frac{1}{2}(n^1 + n^2 + n^3 - 2n^{(I)})\Lambda_I^i = \Gamma\Lambda_I^i \quad (14)$$

where the constant Γ which specifies the isotropic model has been defined above. In particular, we see that the spin connection vanishes for the spatially flat model, and so the Ashtekar connection $A_a^i = \Gamma_a^i + \gamma K_a^i$ is proportional to the extrinsic curvature, whereas in the positively curved model it has an extra term given by the intrinsic curvature of space.

Knowing the spin connection we can express the integrated trace of the extrinsic curvature in terms of the isotropic variables (c, p) :

$$\begin{aligned} K &:= \int d^3x K_a^i E_i^a = \gamma^{-1} \int d^3x (A_a^i - \Gamma_a^i) E_i^a \\ &= \gamma^{-1}(\phi_I^i - \Gamma_I^i)p_i^I = 3\gamma^{-1}(c - \Gamma)p =: K_I^i p_i^I. \end{aligned} \quad (15)$$

We also define the isotropic extrinsic curvature component k by $k\Lambda_I^i := K_I^i = \gamma^{-1}(c - \Gamma)\Lambda_I^i$ such that $K = 3kp$. As proposed in [24], we will use this quantity in order to quantize the Hamiltonian constraint for Lorentzian signature exploiting the relation

$$K = \frac{1}{2}\gamma^{-2}\{H^{(E)}, V\} \text{sgn}(\det a_I^i)$$

which can easily be verified here for the isotropic Euclidean part (13) of the constraint with the symplectic structure (2). This can then be inserted into the Lorentzian constraint

$$H = -H^{(E)} + P \quad (16)$$

with

$$\begin{aligned} P &:= -2(1 + \gamma^2)\kappa^{-1}\det(a_I^i)^{-1}K_{[I}^i K_{J]}^j E_i^I E_j^J \\ &= -(1 + \gamma^2)\kappa^{-1}a^{-3}(K_I^i K_J^j p_i^I p_j^J - K_J^i K_I^j p_i^I p_j^J) \\ &= -6(1 + \gamma^2)\kappa^{-1}a^{-3}k^2 p^2 = -6(1 + \gamma^{-2})\kappa^{-1}(c - \Gamma)^2 \text{sgn}(p)\sqrt{|p|} \end{aligned} \quad (17)$$

to yield the Lorentzian constraint for isotropic models.

3.2 Quantization

According to [22], the Hamiltonian constraint for homogeneous models can be quantized along the lines of the full theory [24] if the special requirements of the symmetry are taken

into account. One arrives at the Euclidean part (note that this corresponds to the relative sign for the two different triad orientations as chosen above; see the discussion following equation (12))

$$\hat{H}^{(E)} = 4i(\gamma\kappa l_P^2)^{-1} \sum_{IJK} \epsilon^{IJK} \text{tr}(h_I h_J h_I^{-1} h_J^{-1} h_{[I,J]}^{-1} h_K [h_K^{-1}, \hat{V}]) \quad (18)$$

where the holonomy operator $h_{[I,J]}$ depends on the symmetry type and is defined by

$$h_{[I,J]} := \prod_K (h_K)^{c_{IJ}^K}.$$

In contrast to [22] we quantized the Poisson bracket of ϕ_I^i and the volume to $-h_K[h_K^{-1}, \hat{V}]$ which is completely along the lines of the full theory. Although in homogeneous models it is possible to use the simpler expression $[h_K, \hat{V}]$, which has been done in [22], this is not advisable as can be seen from a quantization of the inverse scale factor [25]. Therefore, we use here the quantization which is closer to that in the full theory.

Using the extrinsic curvature, the Lorentzian constraint operator can be written as

$$\begin{aligned} \hat{H} &= -\hat{H}^{(E)} + \hat{P} \\ &= -\hat{H}^{(E)} - 8i(1 + \gamma^2)\kappa^{-1}(\gamma l_P^2)^{-3} \sum_{IJK} \epsilon^{IJK} \text{tr} \left(h_I [h_I^{-1}, \hat{K}] h_J [h_J^{-1}, \hat{K}] h_K [h_K^{-1}, \hat{V}] \right) \end{aligned} \quad (19)$$

with (up to ordering ambiguities which will be discussed below)

$$\hat{K} = -\frac{1}{2}i\gamma^{-2}\hbar^{-1} \left[\hat{H}^{(E)}, \hat{V} \right] \widehat{\text{sgn}(\det a_I^i)}. \quad (20)$$

Since \hat{K} appears in \hat{P} within a commutator with holonomies (corresponding to Poisson brackets in the classical expression), the sign $\text{sgn}(\det a_I^i)$ in (20) is important even though \hat{P} is quadratic in \hat{K} .

From the homogeneous operators we can always derive the isotropic ones by inserting holonomies $h_I = \cos(\frac{1}{2}c) + 2\sin(\frac{1}{2}c)\Lambda_I^i \tau_i$ and the isotropic volume operator. Using the dreibein relations (1) for Λ_I^i and $\text{tr}(\Lambda_I) = 0$ one can then take the trace in order to arrive at an operator composed of $\cos(\frac{1}{2}c)$, $\sin(\frac{1}{2}c)$ and \hat{V} . For the Hamiltonian constraint we need

$$\begin{aligned} h_I h_J h_I^{-1} h_J^{-1} &= \cos^4(\tfrac{1}{2}c) + 2(1 + 2\epsilon_{IJ}^K \Lambda_K) \sin^2(\tfrac{1}{2}c) \cos^2(\tfrac{1}{2}c) + (2\delta_{IJ} - 1) \sin^4(\tfrac{1}{2}c) \\ &\quad + 4(\Lambda_I - \Lambda_J)(1 + \delta_{IJ}) \sin^3(\tfrac{1}{2}c) \cos(\tfrac{1}{2}c) \end{aligned}$$

which has been computed using $\Lambda_I \Lambda_J = \frac{1}{2}\epsilon_{IJ}^K \Lambda_K - \frac{1}{4}\delta_{IJ}$. Similarly, we have

$$\begin{aligned} h_K [h_K^{-1}, \hat{V}] &= \hat{V} - \cos(\tfrac{1}{2}c) \hat{V} \cos(\tfrac{1}{2}c) - \sin(\tfrac{1}{2}c) \hat{V} \sin(\tfrac{1}{2}c) \\ &\quad - 2\Lambda_K \left(\sin(\tfrac{1}{2}c) \hat{V} \cos(\tfrac{1}{2}c) - \cos(\tfrac{1}{2}c) \hat{V} \sin(\tfrac{1}{2}c) \right). \end{aligned}$$

These formulae are sufficient in order to derive the Euclidean part of the Hamiltonian constraint for the spatially flat isotropic model

$$\hat{H}^{(E)} = 96i(\gamma\kappa l_P^2)^{-1} \sin^2(\tfrac{1}{2}c) \cos^2(\tfrac{1}{2}c) \left(\sin(\tfrac{1}{2}c) \hat{V} \cos(\tfrac{1}{2}c) - \cos(\tfrac{1}{2}c) \hat{V} \sin(\tfrac{1}{2}c) \right) \quad (21)$$

with action

$$\hat{H}^{(E)}|n\rangle = 3(\gamma\kappa l_P^2)^{-1} \text{sgn}(n) \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) (|n+4\rangle - 2|n\rangle + |n-4\rangle) \quad (22)$$

using (11). Here we see that one can transform to the other sign convention in (12) simply by dropping $\text{sgn}(n)$. At this place it looks unambiguous since for $n = 0$ we have $V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} = 0$, but note that the splitting into the sign and the difference of volume eigenvalues in (11) is ambiguous (since we use $\text{sgn}(0) := 0$, its prefactor is not uniquely defined; in (11) it has just been extended from the general expression for positive and negative n). In quantum geometry only the constraint with sign convention as in (12) can be quantized directly and appears much more natural.

Next we can build the extrinsic curvature operator using the Euclidean part of the Hamiltonian constraint. Since we chose a non-symmetric ordering for the Euclidean constraint, we obtain from (20) a non-symmetric extrinsic curvature operator

$$\begin{aligned} \hat{\mathcal{K}}|n\rangle &= \tfrac{3}{2}i\gamma^{-3}l_P^{-4} \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) \\ &\quad \times \left[\left(V_{\frac{1}{2}(|n+4|-1)} - V_{\frac{1}{2}(|n|-1)} \right) |n+4\rangle - \left(V_{\frac{1}{2}(|n|-1)} - V_{\frac{1}{2}(|n-4|-1)} \right) |n-4\rangle \right] \\ &=: \tfrac{1}{8}il_P^2 (\mathcal{K}_n^- |n+4\rangle - \mathcal{K}_n^+ |n-4\rangle) \end{aligned} \quad (23)$$

where we defined the coefficients

$$\mathcal{K}_n^\pm := \mp 12(\gamma l_P^2)^{-3} \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) \left(V_{\frac{1}{2}(|n\mp 4|-1)} - V_{\frac{1}{2}(|n|-1)} \right) \quad (24)$$

which fulfill $\mathcal{K}_{-n}^- = -\mathcal{K}_n^+$ and are approximately given by $\mathcal{K}_n^\pm \sim n$ for large $|n|$. It is possible to choose a symmetric ordering of $\hat{\mathcal{K}}$ without changing the original ordering of $\hat{H}^{(E)}$, but this is not necessary since we are interested here only in the constraint, which need not be symmetric (in fact, the Euclidean part *must not* be symmetric as we will see below). Nevertheless, we will see shortly that not all orderings for

$$\hat{K}|n\rangle := \alpha \hat{\mathcal{K}} + (1-\alpha) \hat{\mathcal{K}}^\dagger = \tfrac{1}{8}il_P^2 (K_n^- |n+4\rangle - K_n^+ |n-4\rangle) \quad , \quad K_n^\pm = \alpha \mathcal{K}_n^\pm + (1-\alpha) \mathcal{K}_{n\mp 4}^\mp \quad (25)$$

with ordering parameter $\alpha \in \mathbb{R}$ are allowed. Using \hat{K} in some given ordering we obtain the potential term of the Lorentzian constraint

$$\begin{aligned} \hat{P} &= -8i(1+\gamma^2)\kappa^{-1}(\gamma l_P^2)^{-3} \sum_{IJK} \epsilon^{IJK} \text{tr} \left(h_I[h_I^{-1}, \hat{K}] h_J[h_J^{-1}, \hat{K}] h_K[h_K^{-1}, \hat{V}] \right) \\ &= -96i(1+\gamma^2)\kappa^{-1}(\gamma l_P^2)^{-3} \\ &\quad \times \left(\sin(\tfrac{1}{2}c) \hat{K} \cos(\tfrac{1}{2}c) - \cos(\tfrac{1}{2}c) \hat{K} \sin(\tfrac{1}{2}c) \right)^2 \left(\sin(\tfrac{1}{2}c) \hat{V} \cos(\tfrac{1}{2}c) - \cos(\tfrac{1}{2}c) \hat{V} \sin(\tfrac{1}{2}c) \right) . \end{aligned}$$

We already commented on the ordering of \hat{K} , and it will be seen to be crucial to order the operator containing \hat{V} , which quantizes the triad components, to the right.

For \hat{P} we need the action

$$\left(\sin(\tfrac{1}{2}c) \hat{K} \cos(\tfrac{1}{2}c) - \cos(\tfrac{1}{2}c) \hat{K} \sin(\tfrac{1}{2}c) \right) |n\rangle =: -\tfrac{1}{8} l_P^2 (k_n^- |n+4\rangle - k_n^+ |n-4\rangle) \quad (26)$$

introducing

$$k_n^\pm = \tfrac{1}{2} (K_{n+1}^\pm - K_{n-1}^\pm) \quad (27)$$

with $k_n^+ = k_{-n}^-$. Inserting (26), (27) and (24) into the action of \hat{P} demonstrates that expressions for the action of the isotropic Lorentzian constraint can be quite cumbersome, but can be computed explicitly thanks to the completely known volume spectrum (the equation simplifies at large volume where the coefficients k_n^\pm are approximately one, as used in Section 5.2). Fortunately, for the later discussion we will not need the explicit action but only the crucial fact that we can order \hat{K} such that the coefficients k_n^\pm are non-vanishing for all n . In our original operator (23) the coefficients \mathcal{K}_0^\pm and $\mathcal{K}_{\pm 2}^\pm$ vanish leading to $k_{\pm 1}^\pm = 0$ which will be seen in the next section to give a singular evolution. One can easily remedy this by ordering \hat{K} symmetrically which amounts to replacing \mathcal{K}_n^\pm by $\tfrac{1}{2}(\mathcal{K}_n^\pm + \mathcal{K}_{n\mp 4}^\mp)$ and results in coefficients k_n^\pm which never vanish. From now on, we use the ordering

$$\hat{K} := \tfrac{1}{2} (\mathcal{K} + \mathcal{K}^\dagger)$$

such that

$$K_n^\pm = \tfrac{1}{2} (\mathcal{K}_n^\pm + \mathcal{K}_{n\mp 4}^\mp) .$$

Finally, we can compute the action of \hat{P} by using the previously derived operators:

$$\begin{aligned} \hat{P}|n\rangle &= \tfrac{3}{4}(1 + \gamma^{-2})(\gamma \kappa l_P^2)^{-1} \text{sgn}(n) \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) \\ &\times (k_n^- k_{n+4}^- |n+8\rangle - (k_n^- k_{n+4}^+ + k_n^+ k_{n-4}^-) |n\rangle + k_n^+ k_{n-4}^+ |n-8\rangle) . \end{aligned} \quad (28)$$

4 Evolution

Now we have all ingredients for the explicit form of the Hamiltonian constraint equation and can discuss the evolution it governs. For simplicity, we will write down the following formulae for the spatially flat model and will only comment on possible differences in the spatially positively curved model, but most qualitative results apply to both cases.

4.1 Discrete Time

We will use the triad coefficient $p = \text{sgn}(a)a^2$ as internal time which classically makes sense only for positive p . In particular, the evolution breaks down at the classical singularity $p = 0$ so that the two branches $p > 0$ and $p < 0$ are disconnected. (Note that p and

$-p$ result in the same metric², but are not identified by a gauge transformation since the gauge group is $SO(3)$ rather than $O(3)$. Factoring out the large gauge transformation $p \rightarrow -p$ is not allowed since, in particular, it results in a conical singularity at $p = 0$ in the extended phase space which is used in the quantum theory.) This setting enables us to discuss the fate of the singularity in quantum cosmology by studying the evolution close to $p = 0$. For this we need to write the constraint equation $\hat{H}|s\rangle = 0$ for a history $|s\rangle$ as an evolution equation which can only be done in a dreibein, rather than connection, representation since we are using a metrical expression as internal time [29, 13]. According to [23], a dreibein representation is defined by expanding $|s\rangle = \sum_n s_n |n\rangle$ and using the coefficients s_n as a wave function in the dreibein representation. Because of the discreteness of geometric spectra a state in the dreibein representation is a function on a discrete set given by \mathbb{Z} here, and using a metrical internal time implies a discrete time evolution [23]. With our explicit expressions (22), (28) for the Hamiltonian constraint we can write down the difference equations governing the evolution of isotropic models.

In the dreibein representation, the Euclidean part of the constraint acts as

$$(\hat{H}^{(E)}|s\rangle)_n = 3(\gamma\kappa l_P^2)^{-1} \left[\text{sgn}(n+4)(V_{\frac{1}{2}|n+4|} - V_{\frac{1}{2}|n+4|-1})s_{n+4} \right. \\ \left. - 2\text{sgn}(n)(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1})s_n + \text{sgn}(n-4)(V_{\frac{1}{2}|n-4|} - V_{\frac{1}{2}|n-4|-1})s_{n-4} \right]$$

and \hat{P} as

$$(\hat{P}|s\rangle)_n = \frac{3}{4}(1+\gamma^{-2})(\gamma\kappa l_P^2)^{-1} \left[\text{sgn}(n+8) \left(V_{\frac{1}{2}|n+8|} - V_{\frac{1}{2}|n+8|-1} \right) k_{n+8}^+ k_{n+4}^+ s_{n+8} \right. \\ \left. - \text{sgn}(n) \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) (k_n^- k_{n+4}^+ + k_n^+ k_{n-4}^-) s_n \right. \\ \left. + \text{sgn}(n-8) \left(V_{\frac{1}{2}|n-8|} - V_{\frac{1}{2}|n-8|-1} \right) k_{n-8}^- k_{n-4}^- s_{n-8} \right].$$

In a realistic cosmological model we also need matter which enters the evolution equation via its matter Hamiltonian, and we may include a cosmological term. The precise form of the matter and its quantization is not important here, and we will build it into our description by using states $s_n(\phi)$ in the dreibein representation which are functions of the matter degrees of freedom ϕ . Since matter and gravitational degrees of freedom are independent and so commute prior to imposing the constraint, we will get a matter Hamiltonian \hat{H}_ϕ acting on s which is diagonal in the gravitational degree of freedom n for usual matter (for the rare cases of matter with curvature couplings our discussion has to be adapted appropriately; note that our starting point is not an effective Hamiltonian with possible higher curvature terms which would have to be derived only after quantization): $\hat{H}_\phi|n\rangle \otimes |\phi\rangle =: |n\rangle \otimes \hat{H}_\phi(n)|\phi\rangle$. Important for what follows is also that all states $|0\rangle \otimes |\phi\rangle$ are annihilated by the matter Hamiltonian, which is a consequence of special features of quantum geometry. More precisely, all terms in a matter Hamiltonian contain metric components in order to have a scalar density which is integrated to the Hamiltonian; and a

²The author thanks Y. Ma for making him aware of this issue.

quantization of those metric components along [27] leads to an operator annihilating $|0\rangle$, and so $\hat{H}_\phi(0) = 0$. This is analogous to the inverse scale factor which also annihilates $|0\rangle$ and is possible only in quantum geometry because in a matter Hamiltonian both the metric and the inverse metric can appear which cannot simultaneously be zero classically (see [25] for a detailed discussion).

Collecting all ingredients we arrive at the evolution equation

$$\begin{aligned}
& \frac{1}{4}(1 + \gamma^{-2}) \operatorname{sgn}(n + 8) \left(V_{\frac{1}{2}|n+8|} - V_{\frac{1}{2}|n+8|-1} \right) k_{n+8}^+ k_{n+4}^+ s_{n+8}(\phi) \\
& - \operatorname{sgn}(n + 4) \left(V_{\frac{1}{2}|n+4|} - V_{\frac{1}{2}|n+4|-1} \right) s_{n+4}(\phi) \\
& - 2 \operatorname{sgn}(n) \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) \left(\frac{1}{8}(1 + \gamma^{-2})(k_n^- k_{n+4}^+ + k_n^+ k_{n-4}^-) - 1 \right) s_n(\phi) \\
& - \operatorname{sgn}(n - 4) \left(V_{\frac{1}{2}|n-4|} - V_{\frac{1}{2}|n-4|-1} \right) s_{n-4}(\phi) \\
& + \frac{1}{4}(1 + \gamma^{-2}) \operatorname{sgn}(n - 8) \left(V_{\frac{1}{2}|n-8|} - V_{\frac{1}{2}|n-8|-1} \right) k_{n-8}^- k_{n-4}^- s_{n-8}(\phi) \\
& = -\frac{1}{3}\gamma\kappa l_P^2 \operatorname{sgn}(n) \hat{H}_\phi(n) s_n(\phi)
\end{aligned} \tag{29}$$

which, as anticipated in [23], is a difference equation for the coefficients $s_n(\phi)$ in the discrete label n (our discrete time) of order 16 (in [23] the order is higher since the Poisson brackets with the volume have been quantized differently). Note also that due to $k_n^+ = k_{-n}^-$ the equation is symmetric under time reflection $n \mapsto -n$, provided the matter Hamiltonian fulfills $\hat{H}_\phi(n) = \hat{H}_\phi(-n)$.

The gravitational part of the evolution equation is quite complicated and an explicit solution is possible only in simple cases like the Euclidean vacuum equations discussed below. But the equation is amenable to a numerical analysis because it is a difference equation, and given some initial data we can compute subsequent components of the wave function (in a numerical analysis one has to be aware of possible unstable solutions [30]). However, a recursive computation is possible only as long as the highest order coefficient, $\operatorname{sgn}(n + 8) (V_{|n+8|/2} - V_{|n+8|/2-1}) k_{n+8}^+ k_{n+4}^+$, does not vanish. As discussed earlier, we use an ordering of the extrinsic curvature such that k_n^+ never vanishes, but the rest of the coefficient is zero if and only if $n = -8$. This means that, starting at negative n , we can determine components s_n of the history s only up to $n = -1$, and the coefficient for $n = 0$ is not determined by the evolution equation. Because the volume vanishes in the state $|0\rangle$ it seems that as in the classical theory there is a singularity in isotropic models of loop quantum cosmology in which the evolution breaks down. This, however, is not the case as we will show now.

4.2 Fate of the Singularity

We assume that we are given enough initial data for negative n of large absolute value in order to specify all initial conditions for the difference equation of order 16, i.e. we know the wave function $s_n(\phi)$ at 16 successive times n_0 to $n_0 + 15$. From these values we can compute all coefficients of $s_n(\phi)$ for negative n , but for $n = -8$ the highest order

coefficient in (29) vanishes. So instead of determining $s_0(\phi)$ the evolution equation leads to a consistency condition for the initial data: We already know $s_n(\phi)$ for all negative n using (29) for $n \leq -9$, and using the equation for $n = -8$ gives an additional condition between $s_{-16}(\phi)$, $s_{-12}(\phi)$, $s_{-8}(\phi)$ and $s_{-4}(\phi)$. Such a consistency condition is not a problem because it serves to restrict the initial data which is welcome in order to reduce the freedom, and it can be used in order to derive initial conditions from the evolution equation which uniquely fix the semiclassical branch of a wave function [31]. However, we now lack an equation which would give us $s_0(\phi)$ in terms of the initial data seemingly leading to a breakdown of the evolution as mentioned above. But the situation is much better: We cannot determine $s_0(\phi)$ because it drops out of the evolution equation, but it also does not appear in the equations for $n > -8$. Therefore, we can compute all coefficients for positive n and in this sense we can evolve through the classical singularity. At this point we used the crucial fact $\hat{H}_\phi(0) = 0$, which naturally holds in quantum geometry; otherwise, $s_0(\phi)$ would enter the evolution equation via the matter part.

Of course, in order to determine the complete state $|s\rangle$ we also need to know s_0 which, as we will show now, can be fixed independently of the evolution. First we note that there is always a trivial, degenerate solution to the constraint equation given by $s_n(\phi) = \delta_{0,n}s_0(\phi)$ which is completely supported on degenerate metrics and which is a true eigenstate of the constraint with eigenvalue zero. In the vacuum case, it corresponds to the classical solution $p = 0$ which is of no physical interest, but with matter there can be no classical analog because this solution arises only due to $\hat{H}_\phi(0) = 0$ whereas the classical matter Hamiltonian usually diverges for $p = 0$. All other solutions are orthogonal to the degenerate solution and, therefore, must have $s_0(\phi) = 0$ demonstrating that in an evolving solution this coefficient is fixed from the outset and we can determine the complete state using the evolution equation (in a given solution to the constraint equation there can be an arbitrary admixture of the degenerate state, but it does not affect the solution at non-zero n). After this discussion, one can absorb the sign factors in (29) into the wave function, which had been done in [26, 31] for simplicity. This is free of ambiguities here for evolving solutions where we use the condition $s_0 = 0$; compare the remarks after (22).

We have now shown that the evolution equation (29) does not break down at the classical singularity, and in this sense there is no singularity in loop quantum cosmology. But in general a state will be supported on the degenerate states $|\pm 1\rangle$ in which the volume vanishes. Although this may look problematic, the inverse scale factor, whose classical divergence is responsible for the curvature singularity, remains *finite* in these states. This feature of quantum geometry, which also was very crucial in our proof of the absence of the singularity because it implied a vanishing matter Hamiltonian in $|0\rangle$, is the fundamental deviation from classical geometry leading to the consequences discussed in the present article. While we used this general property of the matter Hamiltonian, the precise form of matter is irrelevant and so our conclusion remains true for any standard type of matter with or without a cosmological constant, and also for the spatially positively curved model.

On the other hand, the factor ordering of the constraint is very crucial, for in a different ordering the coefficient $s_0(\phi)$ would not completely drop out of the evolution and we would not have the degenerate solution. Ordering the triad components to the left rather than

to the right results in a coefficient $\text{sgn}(n)(V_{|n|/2} - V_{|n|/2-1})$ of s_{n+k} replacing all $\text{sgn}(n+k)(V_{|n+k|/2} - V_{|n+k|/2-1})$ in (29). The highest order coefficient then vanishes first for $n = 0$ so that s_8 remains undetermined and will *not* drop out of the equation for positive n . This results in s_{12}, \dots depending on s_8 , and we no longer have a solution similar to the completely degenerate state $s_n = s_0 \delta_{n0}$. Also, we must not use a symmetric ordering since in this case the highest order coefficient $\text{sgn}(n)(V_{|n|/2} - V_{|n|/2-1}) + \text{sgn}(n+8)(V_{|n+8|/2} - V_{|n+8|/2-1})$ vanishes for $n = -4$ and s_4, s_8, \dots remain undetermined by initial data (for different reasons not to use a symmetric ordering of the Hamiltonian constraint in quantum general relativity see [32]). Thus, a non-singular evolution of the observed kind, which is possible only for one of the three standard orderings (triads to the left or right, and the symmetric ordering) may be used as a criterion to fix the factor ordering ambiguity of the Hamiltonian constraint. The ordering derived here corresponds to the one chosen in [24] for the constraint in the full theory.

There are non-symmetric orderings of the constraint for which the highest (and lowest) order coefficient never vanishes. With such an ordering there would be no state corresponding to the classical solution $p = 0$ in the vacuum case, and a general evolving solution would be supported on the degenerate state $|0\rangle$ with the s_n depending on s_0 . Since this state plays a special role even kinematically (recall that quantizations of both the scale factor and its inverse annihilate it [25]), a special behavior of any evolving state, like the orthogonality to it described above, is preferable. More importantly, a vanishing highest order coefficient implies a consistency condition which poses initial conditions on evolving states. As we will see in Sec. 5.1, the unique state corresponding to flat Euclidean space only results with this condition (see also [31] for the case with matter). Non-vanishing highest order coefficients are also obtained for a symmetric ordering if one first transforms to the alternative sign convention in (22). But recall that this transformation is not free of ambiguities right at the value $n = 0$ which is important for a discussion of the singularity. Thus the choice of this ordering is problematic. The scenario of [26, 31] and the present paper is realized in *only one* ordering of the constraint, with triads to the right, which will always be used from now on. This ordering has been used previously in order to derive consistency of the formal constraints [33]. (However, the Chern–Simons state, which has been found as a solution to the formal Euclidean Hamiltonian constraint with a positive cosmological constant, requires the opposite ordering [34]. But since there is no physical correspondence of this state it is not necessary to find it as a solution, and so its disappearance does not present an argument against an ordering; for the Lorentzian constraint it disappears, anyway.)

Intuitively, we have the following picture of an evolving universe: For negative times n of large absolute value we start from a classical universe with large volume. It contracts ($V_{(|n|-1)/2}$ decreases with increasing negative n) to reach a degenerate state of zero volume, classically seen as a singularity, in which it bounces off in order to enter an expanding branch and to reach again a classical regime with large volume. The change of sign in p during the bounce means that the universe “turns its inside out” there [35]. A possible recollapse and an iteration of this behavior depends on the matter content, but for the evolution close to the singularity matter is irrelevant. What remains to show is that for

large volume we have in fact the correct semiclassical behavior, to which we turn now.

4.3 Semiclassical Regime

Our evolution equation (29) is of the order 16 for the spatially flat model and even 20 for the positively curved model, and so there are many independent solutions (in fact, there are infinitely many independent solutions if we take into account the matter degrees of freedom, but we are mostly interested in the freedom coming from the sole gravitational variable n). Of course, a classical cosmological model does not have so many independent solutions, and so most of the quantum solutions cannot have a classical counterpart. In the present section we investigate the conditions for a solution to have a semiclassical branch. (This issue is discussed in more detail in [31].)

We first have to define conditions for a semiclassical regime. Obviously, the volume should be large compared to the Planck scale and components of the curvature should be small. Moreover, continuous space-time has to be a very good approximation to the discrete space and time of quantum geometry. The first condition of large volume is straightforwardly implemented by requiring $|n|$ to be large, but the second condition for the curvature is more problematic. At this point we have to recall that we are studying isotropic, in particular homogeneous, models which are represented by idealized, distributional states in the full quantum theory. Such an idealization can lead to problems because one only has access to curvature integrated over space rather than local curvature components. In the present context, we may have to face infrared problems in the large volume regime because the product of curvature and volume of space may be large even if the local curvature is small. For instance, if we have a positive cosmological constant Λ , it will enter the wave function in the dimensionless combination Λp which diverges for $p \rightarrow \infty$, even though the local curvature scale given by Λ may be small. Similarly, in the positively curved model we have the connection coefficient $c = \frac{1}{2} + \gamma k$ where $\Gamma = \frac{1}{2}$ comes from the spin connection and has the meaning of the integrated intrinsic curvature of space. Therefore, even if the extrinsic curvature k is small enough, c may not be so. We will evade those infrared problems by assuming c to be small when studying the semiclassical limit. For the flat model this can always be achieved by choosing not too large p .

Furthermore, contrary to a classical symmetry reduction in which a homogeneous geometry can be slightly perturbed by adding small non-homogeneous modes, homogeneous quantum states are distributional and can only be approximated in the weak topology of the kinematical Hilbert space. A consequence is the level splitting in the volume spectrum if we break a symmetry: the simple isotropic volume spectrum becomes increasingly complicated as in the homogeneous case or in the full theory. In particular, whereas the isotropic volume spectrum has an increasing level distance for large j , the full volume spectrum becomes almost continuous (similarly as discussed for the area spectrum in [16]). Such an almost continuous spectrum makes the transition to a classical geometry with its continuous volume obvious; but for this also a spectrum with decreasing *relative* level distance is sufficient, as is the case in isotropic models (compare with the equidistant energy spectrum of the harmonic oscillator which does not prevent the correspondence to a

continuous energy spectrum in the classical regime for large energies). So compared to a given volume, the change caused by increasing the time n to $n + 1$ is always negligible and cannot be detected by a classical observer.

We incorporate this observation in our main condition (*pre-classicality* [31]) for a semiclassical regime: the wave function $s_n(\phi)$ must not depend strongly on n in the large volume regime in order to be regarded as being semiclassical there. More precisely, we demand that it is possible to interpolate between the discrete labels n and define a wave function $\psi(a) := s_{n(a)}$ with $n(a) := 6 \operatorname{sgn}(a) a^2 \gamma^{-1} l_P^{-2}$ with a ranging over a continuous range (using $|a| = \sqrt{|p|} = \sqrt{\gamma} l_P \sqrt{|n|/6}$ for large $|n|$ as interpolation points) which varies only on scales much larger than the Planck scale. At this point we may have to face the above mentioned infrared problems: a cosmological constant leads to a wave function with wave length $(\Lambda a)^{-1}$ which inevitably becomes smaller than the Planck length for large a . Generically, there should be a regime in which curvatures are small and the volume is not too large in order to allow a continuous time approximation $\psi(a)$.

Given a wave function $\psi(a)$ interpolating the discrete function s_n , we can approximate the action of the Hamiltonian constraint by derivative operators. The basic operators are the difference operator $\Delta = 2i \sin \frac{1}{2}c$ and the mean operator $\mu = \cos \frac{1}{2}c$ which have the leading order action

$$(\Delta s)_{n(a)} = s_{n(a)+1} - s_{n(a)-1} = \frac{\gamma l_P^2}{6a} \frac{d\psi}{da} + O(l_P^5/a^5) \quad (30)$$

and

$$(\mu s)_{n(a)} = \frac{1}{2}(s_{n(a)+1} + s_{n(a)-1}) = \psi(a) + O(l_P^4/a^4) \quad (31)$$

following from a Taylor expansion. The higher order corrections also contain higher derivatives, but in the semiclassical regime we only need the leading order resulting in the standard Wheeler–DeWitt operator

$$\kappa \hat{H}^{(E)} \sim -96(i\Delta/2)^2 \cdot \frac{1}{4}a \sim -6 \left(-\frac{1}{3}i\gamma l_P^2 \frac{d}{d(a^2)} \right)^2 a$$

for large a where we inserted Δ and $\mu \sim 1$ in (21), used (11) and expanded the volume eigenvalues in $j \sim 3a^2 \gamma^{-1} l_P^{-2}$. This is exactly what one obtains from the classical constraint

$$\kappa H^{(E)} = -6c^2 \operatorname{sgn}(p) \sqrt{|p|}$$

in standard quantum cosmology by quantizing $3\hat{c} = -i\gamma l_P^2 d/dp$. In our framework, however, this is only an approximate equation valid for large scale factors where a continuous time approximation of the discrete time wave function is possible. Analogously, one can show that the term \hat{P} in the Lorentzian constraint has the correct behavior semiclassically which is also true for the spatially positively curved model. For the Euclidean part of the constraint, this can most easily be seen in the connection representation where the above expansion of the difference operator corresponds to an expansion of $\sin \frac{1}{2}c$ in c . Thus, by construction of the Hamiltonian constraint [22] an expansion will result in the standard

quantum cosmology expression at leading order. This observation also shows why small c are important in the semiclassical regime.

Arrived at the standard quantum cosmology framework, one can use WKB-techniques in order to derive the correct semiclassical behavior. This demonstrates, ignoring possible infrared problems, that isotropic models with the evolution equation (29) have the correct semiclassical behavior for large volume which is achieved in a two-step procedure [36]: First, the discrete time behavior has to be approximated by introducing a continuous time and interpolating the wave function which results in standard quantum cosmology. In a second step, one can perform the classical limit in order to arrive at the classical description. Since at fixed κ and \hbar the parameter γ determines the scale of the discreteness, one can also describe this by a two-fold limit $\gamma \rightarrow 0$, $n \rightarrow \infty$ followed by $\hbar \rightarrow 0$.

In this picture, a universe is fundamentally described quantum geometrically in a discrete time, and standard quantum cosmology only arises as an approximation which is not valid close to the singularity. This explains the large discrepancies of standard quantum cosmology and loop quantum cosmology regarding the fate of the singularity. Also the issue of choosing boundary conditions, which are usually imposed at $a = 0$ in standard quantum cosmology, appears in a different light. In fact, our discrete time evolution can be seen to lead to dynamical initial conditions which are derived from the evolution equation and not imposed independently [31].

Moreover, using higher order corrections in (30) and (31) and in the expansion of the volume eigenvalues one can derive perturbative corrections to the standard Wheeler–DeWitt operator. Thereby, one obtains an effective Hamiltonian containing higher curvature and higher derivative terms. The closer one comes to the classical singularity, the more of those perturbative corrections are necessary, until such a description completely breaks down at the classical singularity. Because we know the non-perturbative equation which is discrete in time, we can see that a perturbative formulation cannot suffice: even if one knew all perturbative corrections, it would be very hard to see how they add up to the discrete time behavior without knowing the non-perturbative formulation. Furthermore, we see that a non-locality in time caused by the discreteness is responsible for higher order corrections. This also gives an indication as to why general relativity is perturbatively non-renormalizable: adding local counterterms to a local action can never result in a non-local behavior like that observed above.

5 Quantum Flat Space

As we have seen, the complete Lorentzian constraint is of an awkward form which makes it complicated to find explicit solutions. Nevertheless, for the spatially flat model it is quite simple at large volume, where the coefficients containing differences of volume eigenvalues are nearly identical. The Euclidean part is then of the form of a squared difference operator, whereas the Lorentzian constraint is effectively of fourth order. For a complete solution we also need to take into account the behavior at small volume, and we will demonstrate for the Euclidean part that its values at the classical singularity are crucial for the cor-

respondence with the classical situation. Recall that classically we have two solutions in the vacuum case (Appendix A), a degenerate one given by $p = 0$ and Euclidean four-space characterized by $c = 0$ (vanishing extrinsic curvature). Standard quantum cosmology leads to two independent non-degenerate solutions $\xi_1(c) = \delta(c)$ and $\xi_2(c) = \delta'(c)$ in the connection representation only one of which corresponds to Euclidean space. Moreover, there are problems in standard quantum cosmology because it is not possible to invert triad operators, even though there is no classical singularity in flat space.

5.1 Quantum Euclidean Space

We have already shown that well-defined quantizations of inverse triad operators do exist in loop quantum cosmology, so that we do not have to deal with the second problem. The first problem of too many solutions will now be investigated for the simplest model, the vacuum Euclidean constraint with flat spatial slices. At first sight, it seems to be more severe because the discrete Euclidean evolution equation is of order eight, so we have to expect eight independent solutions. We already know that one of them is the degenerate solution $s_n = s_0 \delta_{n,0}$ corresponding to $p = 0$, and we have to study the remaining seven solutions which all lie in the continuous part of the spectrum of the constraint. Since we are only interested in solutions with classical regimes we also impose our condition for pre-classical behavior, namely that the wave function s_n does not vary strongly from n to $n + 1$ for large $|n|$. This condition, which is the only one besides the evolution equation, ensures the possibility of semiclassical behavior for large volume and is independent of the explicit form of classical solutions.

We have the difference equation

$$\begin{aligned} 0 = & \operatorname{sgn}(n+4) \left(V_{\frac{1}{2}|n+4|} - V_{\frac{1}{2}|n+4|-1} \right) s_{n+4} - 2 \operatorname{sgn}(n) \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) s_n \\ & + \operatorname{sgn}(n-4) \left(V_{\frac{1}{2}|n-4|} - V_{\frac{1}{2}|n-4|-1} \right) s_{n-4} \end{aligned} \quad (32)$$

which can immediately be seen to split into independent equations for the four sequences s_{4m} , s_{4m+1} , s_{4m+2} , and s_{4m+3} with $m \in \mathbb{Z}$. The first sequence contains the classical singularity at $m = 0$ and is subject to the consistency condition arising from the vanishing highest order coefficient for $n = -4$. Therefore, it has only one independent solution (the would-be other one is the degenerate solution), whereas the three other sequences all have two independent solutions because they are subject to a difference equation of order two with never vanishing coefficients. By sticking together arbitrary solutions for all four series we get all the seven independent non-degenerate solutions of (32). At this point, we can already impose our selection criterion of pre-classical behavior for large volume: In this regime, all four series have solutions $s_{4m+i} \sim a_i(4m+i) + b_i$, $i = 0 \dots 3$, with an additional consistency condition relating a_0 and b_0 which can only be determined in the small volume regime. These solutions can be seen by noting that for large $|n|$ the coefficients of s_{n+4} , s_n , and s_{n-4} in (32) are nearly identical. Our classicality condition then tells us that $a_0 = a_1 = a_2 = a_3 =: a$ because otherwise the complete solution would vary strongly for

large $|n|$ when jumping between the four series: e.g., $s_{4m+1} - s_{4m} = 4(a_1 - a_0)m + b_1 - b_0$ becomes arbitrarily large for large $|m|$ if $a_1 - a_0 \neq 0$. Furthermore, the coefficients b_i cannot be very different from each other for the same reason where the difference $b_i - b_j$ affects the amplitude but not the wave length of the variation in the wave function. According to our condition that there must not be a variation at the Planck scale, regardless of the amplitude, we also have to set $b_0 = b_1 = b_2 = b_3 =: b$ (one may permit differences in the b_i bounded by some small parameter ϵ , but this will only lead to the solution with identical b , which is interpreted as the semiclassical part, together with small non-pre-classical contributions). Therefore, the classicality condition reduces the eight parameters a_i, b_i to only two parameters a and b determining the form $s_n = an + b$ for large $|n|$ without reference to a particular classical solution. Now we are in a position similar to that of standard loop quantum cosmology: we have two independent solutions only one of which can correspond to classical Euclidean four-space. But we still have the consistency condition relating a and b which reduces the two independent solutions to only one. To find this unique non-degenerate solution with pre-classical behavior we have to use the full equation (32) also in the small volume regime and in fact right at the classical singularity. This regime is, as demonstrated in the preceding section, not accessible to standard quantum cosmology which explains the fact that there are too many solutions in this approach. However, it is not guaranteed that the unique solution corresponds to the classical solution $c = 0$ which can only be decided when we know its explicit form. Since we need the evolution equation at the singularity for a complete solution which also affects the large volume behavior by fixing the relation between a and b , we can perform a crucial test of loop quantum cosmology for very strong fields by comparing its unique solution with the classical solution at large volume.

The consistency condition only appears for the sequence s_{4m} on which we can focus from now on; the remaining three sequences are then fixed by the pre-classicality condition. We first look at the branch for $m > 0$ where we choose the only free parameter s_4 : whereas the coefficient $s_0 = 0$ is fixed (or drops out if non-zero), all other coefficients are determined by (32) which can be solved for the highest order component

$$s_n = \operatorname{sgn}(n) \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right)^{-1} \left[2 \operatorname{sgn}(n-4) \left(V_{\frac{1}{2}|n-4|} - V_{\frac{1}{2}|n-4|-1} \right) s_{n-4} - \operatorname{sgn}(n-8) \left(V_{\frac{1}{2}|n-8|} - V_{\frac{1}{2}|n-8|-1} \right) s_{n-8} \right]$$

when $n \neq 0$. For positive $n = 4m$, $m \in \mathbb{N}$, we obtain successively

$$\begin{aligned} s_8 &= 2 \frac{V_2 - V_1}{V_4 - V_3} s_4, \\ s_{12} &= \frac{2(V_4 - V_3)s_8 - (V_2 - V_1)s_4}{V_6 - V_5} = 3 \frac{V_2 - V_1}{V_6 - V_5} s_4 \end{aligned}$$

and so on, leading by induction to

$$s_{4m} = |m| \frac{V_2 - V_1}{V_{2|m|} - V_{2|m|-1}} s_4. \quad (33)$$

For negative n we can do the same, leading to s_{-4}, s_{-8}, \dots in terms of s_4 . The result is (33), now with arbitrary $m \in \mathbb{Z}$, which is the exact solution for the sequence s_{4m} and automatically fulfills the consistency condition since we started from $s_0 = 0$. Implicitly, (33) determines the relation between a and b such that we now also have the unique solution with pre-classical behavior given by

$$s_n = \frac{1}{4}|n| \frac{V_2 - V_1}{V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1}} s_4. \quad (34)$$

Dropping constant factors (or choosing $s_4 := 2(V_2 - V_1)^{-1}$), this yields in the connection representation

$$\psi(c) = \sum_{n \in \mathbb{Z}} s_n |n\rangle = \sum_{j=0}^{\infty} \frac{2j+1}{V_{j+\frac{1}{2}} - V_{j-\frac{1}{2}}} \zeta_j(c) \quad (35)$$

where the expression $2j+1 = |n|$ (rather than another linear function in j) appears because the consistency condition fixed the relation between a and b . This allows us to check the compatibility of this condition, which arose because of the structure at the classical singularity, with the correct classical behavior: we expect a solution which is related to the δ -function in c incorporating the classical solution $c = 0$ (see also App. A).

More precisely, since we chose an ordering with the triad components to the right in the connection representation, which has been seen to be necessary in order to remove the singularity, we should expect a quantization of $a = \text{sgn}(p)\sqrt{|p|}$ to map ψ to the delta function (the classical constraint is $-6c^2 \text{sgn}(p)\sqrt{|p|}$ in the ordering chosen for the quantization). A possible quantization of a maps

$$\hat{a}\zeta_j = 2i(\gamma l_P^2)^{-1}(V_{j+\frac{1}{2}} - V_{j-\frac{1}{2}})\chi_j$$

with an analogous action on χ_j , which has the correct large- j behavior for $\sqrt{|p|}$ and which maps ζ_j to $i\chi_j$ (and to zero for $j = -\frac{1}{2}$). The last property is necessary due to the $\text{sgn}(p)$ which can be seen from the action on $|n\rangle$. One can also use the techniques of [25] in order to derive this quantization: writing

$$\text{sgn}(p)\sqrt{|p|} = a = \frac{1}{3}\Lambda_i^I a_I^i = -\frac{2}{3}\text{tr}(\Lambda^I a_I^i \tau_i)$$

and using Thiemann's quantization of the co-triad components we have

$$\hat{a} = -\frac{4}{3}i(\gamma l_P^2)^{-1} \sum_I \text{tr}(\Lambda^I h_I [h_I^{-1}, \hat{V}]) = -4i(\gamma l_P^2)^{-1} \left(\sin(\frac{1}{2}c) \hat{V} \cos(\frac{1}{2}c) - \cos(\frac{1}{2}c) \hat{V} \sin(\frac{1}{2}c) \right)$$

acting as

$$\begin{aligned} \hat{a}\chi_j &= -2i(\gamma l_P^2)^{-1}(V_{j+\frac{1}{2}} - V_{j-\frac{1}{2}})\zeta_j \\ \hat{a}\zeta_j &= 2i(\gamma l_P^2)^{-1}(V_{j+\frac{1}{2}} - V_{j-\frac{1}{2}})\chi_j. \end{aligned} \quad (36)$$

The eigenvalues of \hat{a} are

$$a_j = \pm 2(\gamma l_P^2)^{-1}(V_{j+\frac{1}{2}} - V_{j-\frac{1}{2}})$$

which for large j is

$$|a_j| \sim \sqrt{\frac{1}{3}\gamma l_P^2 j} \sim V_j^{\frac{1}{3}}.$$

Applying \hat{a} of (36) to our solution (35) yields

$$\hat{a}\psi(c) = 2i(\gamma l_P^2)^{-1} \sum_j (2j+1) \chi_j(c) = 2i(\gamma l_P^2)^{-1} \delta(c)$$

which in fact is proportional to the δ -function on the configuration space $SU(2)$. For this it is crucial that we have the factor $2j+1$ which appears uniquely only if one uses the consistency condition arising from the behavior at the classical singularity. Thus, the unique solution to the Euclidean constraint with semiclassical behavior in spatially flat isotropic loop quantum cosmology correctly corresponds to Euclidean four-space with vanishing extrinsic curvature. Similarly in other models, the consistency condition together with the pre-classicality condition on the variation of the wave function for large a always selects a unique solution. In this way *dynamical initial conditions* are derived from the evolution equation [31] and not imposed ad hoc as usually done in standard quantum cosmology.

5.2 Lorentzian Constraint at Large Volume

For large $|n|$ the Lorentzian constraint equation (29) simplifies since $V_{|n+k|/2} - V_{(|n+k|-1)/2}$ is approximately independent of k for $n \gg k$ and the extrinsic curvature coefficients k_n^\pm are nearly one. Introducing $t_m := s_{2m}$, the vacuum constraint equation takes the form

$$\begin{aligned} 0 &= \frac{1}{4}(1 + \gamma^{-2})t_{m+4} - t_{m+2} + \frac{1}{2}(3 - \gamma^{-2})t_m - t_{m-2} + \frac{1}{4}(1 + \gamma^{-2})t_{m-4} \\ &= \frac{1}{4}[(\Delta^4 + 4\gamma^{-2}\Delta^2\mu^2)t]_m \\ &= \frac{1}{4}[\Delta^2(\Delta + 2i\gamma^{-1}\mu)(\Delta - 2i\gamma^{-1}\mu)t]_m \end{aligned}$$

using again the central difference and mean operators Δ and μ . Because they commute we can split this equation into

$$\begin{aligned} \Delta^2 t &= 0 \\ \text{or } (\Delta + 2i\gamma^{-1}\mu)t &= 0 \\ \text{or } (\Delta - 2i\gamma^{-1}\mu)t &= 0 \end{aligned}$$

with independent solutions

$$\begin{aligned} t_m^{(1)} &= c_1, \quad t_m^{(2)} = c_2 m \\ t_m^{(3)} &= c_3 \left(\frac{1 - i\gamma^{-1}}{1 + i\gamma^{-1}} \right)^m, \quad t_m^{(4)} = c_4 \left(\frac{1 - i\gamma^{-1}}{1 + i\gamma^{-1}} \right)^{-m}. \end{aligned}$$

For $\gamma = 1$ we can also use the form

$$t_m^{(3)} = c_3 \operatorname{Re}(i^m) = \cos(m\frac{\pi}{2}), \quad t_m^{(4)} = c_4 \operatorname{Im}(i^m) = \sin(m\frac{\pi}{2}).$$

As with the Euclidean constraint we have still more solutions since the original equation (29) is of order 16. But again it splits into four sequences with solutions as above which can be put together to form all 16 independent solutions. Thanks to the pre-classicality condition of mild variation only four of them are relevant. However, only two, $t^{(1)}$ and $t^{(2)}$, can correspond to the two solutions of the second order standard Wheeler–DeWitt equation; the rest has to be excluded on general grounds which again are provided by pre-classicality. This immediately excludes $t^{(3)}$ and $t^{(4)}$ if $\gamma = 1$ which jump between the values 0 and ± 1 , and also for $\gamma \neq 1$ if γ is of order one or less (which is true for the physical value [37, 38]): $t_m^{(3)}$ and $t_m^{(4)}$ are of the form $\exp(\pm im\theta)$ with $\theta = \arccos[(1 - \gamma^{-2})/(1 + \gamma^{-2})]$ which is $\pi > \theta > \frac{\pi}{2}$ for $0 < \gamma < 1$.

We now arrived at two independent solutions allowed for a semiclassical analysis from which a particular combination is selected by the consistency condition at the classical singularity. To evaluate this we would need to take into account the exact equation (29) also for small volume, from which we refrain here. This appears not to be possible analytically in closed form, but can easily be done in a numerical study. Nevertheless, it is easy to see that the Hamiltonian constraint equation has solutions of the same semiclassical behavior for all values of γ , which contradicts the hope [39] that the Hamiltonian constraint equation selects a value for γ . We can only conclude that a large parameter $\gamma \gg 1$ would lead to additional pre-classical solutions lacking any correspondence to a classical solution (e.g., oscillating solutions for flat space). This may be taken as an argument that γ cannot be much larger than one, in coincidence with [37, 38].

6 Comparison with Other Approaches

A resolution or avoidance of the classical singularity has been claimed before in a variety of approaches. After the singularity theorems of general relativity [1] had been established, it became clear that one has to couple matter which violates energy conditions in order to evade them (it is sufficient to violate only the strong energy condition [5]). This can be achieved with either classical [2] or quantum matter [3, 4] leading to a bounce in the evolution of a universe at positive radius. However, this conclusion is model and parameter dependent and, therefore, not a generic behavior. Furthermore, the threat of a singularity is still present in gravity, but only avoided by particular types of matter (and, since quantum matter field theories have their own divergences, it may be dangerous to call upon quantum matter for a rescue from the singularity).

Another idea to evade the singularity theorems consists in changing general relativity. Since its action is deemed to be only an effective action of something more fundamental, there can be correction terms being non-linear in the Ricci scalar R . Inclusion of the lowest order correction quadratic in R has been shown to yield solutions which do not encounter a singularity [6, 7, 8]. Again, the conclusion is parameter dependent and, in fact, inconsistent because the non-singular solutions emerge only as artifacts of the truncation of the higher order corrections [9]. This situation suggests that a complete non-perturbative formulation is necessary for an investigation of the fate of the classical singularity.

The original approach to this problem in canonical quantum gravity, which is non-perturbative, was started in [10]. Here, it was proposed that one should use the boundary condition $\psi(0) = 0$ of a vanishing wave function right at the classical singularity. It has also been speculated that this condition is enforced by an ad hoc Planck potential which is relevant only for small scale factors [40]. However, as argued in [12], this requirement by itself cannot be regarded as a sufficient condition for the absence of a singularity because the scale factor has a continuous spectrum in standard quantum cosmology (note that in loop quantum cosmology the spectrum of the scale factor is discrete, but the mechanism which removes the classical singularity is very different from DeWitt’s proposal); in addition an appropriate fall-off behavior of ψ close to $a = 0$ would be necessary. In this context, it has also been suggested, sometimes for purely mathematical reasons in order to obtain a self-adjoint id/dp , to extend minisuperspace to include negative volumes, which would remove the boundary at $a = 0$ and allow wave functions to extend into this regime [34] (although this may seem similar to the evolution through the singularity derived in the present paper, it is not to be confused with our negative p which still leads to *positive* volume: in contrast to negative definite metrics, negative triads are allowed classically even though disconnected from the $p > 0$ sector if one requires non-degeneracy). The negative metric branch lacks a classical interpretation, and so the wave function is completely quantum without semiclassical interpretation in this large region of the configuration space. It has been suggested that the transition to negative volume should be interpreted as a signature change to Euclidean space-time [41] or a “tunneling from nothing” [42].

As derived in this paper, loop quantum cosmology is able to describe the behavior of a universe close to the classical singularity. It always leads to a decoupling of s_0 from solutions of cosmological behavior, reminiscent of DeWitt’s $\psi(0) = 0$. However, since from the present perspective standard quantum cosmology completely breaks down in this regime, a condition for the standard wave function $\psi(a)$ is no longer meaningful at $a = 0$. This condition for s_0 is in fact important for the absence of a singularity, and it serves to select a unique superposition of the two WKB components when evolved into the semiclassical regime [31]. At $a = 0$ we have a transition to another branch which opens to large *positive* volume at *negative* time (rather than a “tunneling from nothing”, our picture of an evolving universe could be described as “tunneling through nothing” if one wants to identify “nothing” with the degenerate state $|0\rangle$).

This picture of a branch preceding the classical singularity is reminiscent of the “pre-big-bang” scenario (and other, more recent constructions) of string cosmology [43, 44] where a contracting universe preceding the singularity has been claimed which should be connected to the present expanding branch through a high curvature regime. However, lacking a non-perturbative framework, this claim cannot be substantiated at present.

The possibility of an evolution through a degenerate state also reminds of results which have been obtained in the context of mirror symmetry: by mapping the degenerate state to an equivalent non-degenerate one it is possible to extend the evolution through a singular geometry [45, 46]. However, this has been demonstrated only for very special spaces where one generally focuses on the geometry of compact directions; these spaces are not sufficiently realistic to be of direct physical interest, let alone cosmological models.

7 Conclusions

A reduction of quantum geometry to isotropic geometries leads to models in which explicit computations are possible, thanks primarily to the completely known volume spectrum. Therefore, they provide an ideal test arena for the techniques of quantum geometry, which turn out to work without any problems. Moreover, they are interesting in their own right as cosmological models where they shed light on certain aspects of the classical singularity which were not illuminated in any other approach to (quantum) cosmology. A kinematical indication for a better behavior of loop quantum cosmology close to the classical singularity comes from a quantization of the inverse scale factor [25] using techniques for the quantization of matter Hamiltonians to densely defined operators in quantum geometry [27]. The result is a bounded inverse scale factor which does not diverge even if the volume is zero, a result which is possible only in a quantum theory of geometry. In the present paper we established the absence of a singularity by studying evolution equations at the dynamical level: whereas classically the evolution breaks down at the singularity, in loop quantum cosmology we can evolve through it. Since evolution through a degenerate state is possible, one could also obtain topology change in quantum geometry.

At this point we explain in more detail in which sense the singularity is absent in loop quantum cosmology. One might think that there is still a singular space geometry of vanishing volume. But this is not as problematic as in the classical theory since, e.g., the inverse scale factor does not diverge. One should also keep in mind that vanishing of volume is possible even classically without a singularity: it may just signal the presence of a horizon as is the case in (non-singular) de Sitter space-time when sliced by flat spaces. In this case one can, of course, evolve through the horizon by choosing an appropriate time coordinate. In contrast to a singular space-time, such a manifold is not geodesically incomplete. On the other hand, the existence of an incomplete curve together with energy conditions for the matter inevitably leads to a curvature singularity [1]. At such a point, the curvature tensor cannot even be interpreted in a distributional sense and so Einstein's field equations break down. There is then no means to extend the singular space-time beyond the singularity in a unique manner (it may be possible to extend a space-time continuously, but never uniquely). The evolution equation (29) of isotropic loop quantum cosmology, on the contrary, never breaks down and so always gives rise to a unique extension through the quantum regime containing the classical singularity.

In deriving this behavior it was our strategy always to be as close to the full theory as possible, e.g. when quantizing the Hamiltonian constraint. Although one might have simplified some expressions in a model-dependent way, this would have led to deviations from the methods of the full theory. For instance in the case of flat spatial slices the classical Lorentzian constraint and its Euclidean part only differ by a factor γ^{-2} so that one might be tempted to use this relation also in a quantization which would strongly simplify the quantum constraint. However, this fact crucially depends on i) $K_a^i \propto A_a^i$ (due to $\Gamma_a^i = 0$) and ii) $\epsilon_{ijk} A_a^i A_b^j \propto F_{ab}^k$ (due to $dA = 0$) both of which fail in other homogeneous models, let alone in the full theory. Making use of these relations would simplify the computation, but the results were not trustworthy since the contact to the

full theory would have been lost. Note that in standard quantum cosmology one does not have a corresponding quantization of the full theory as guidance, and thus lacks means to evaluate manipulations. In fact, loop and standard quantum cosmology differ from each other right in the regime where quantum gravitational effects are important. Standard quantum cosmology uses quantum mechanical methods and phenomena (like the tunneling effect) but not full quantum gravity, whereas loop quantum gravity is close to the full theory of quantum geometry. Some of its quantization techniques may seem to be unfamiliar from the viewpoint of quantum mechanics, but they are necessary since analogous techniques are required for a consistent quantization of gravity. Moreover, quantization ambiguities (like the one described at the beginning of this paragraph) are severely restricted by requiring that analogous quantizations must be possible in the full theory.

For the absence of a singularity the form of the matter coupled to gravity is irrelevant because the removal of the singularity is completely due to quantum geometry. On the other hand, the (non-symmetric) factor ordering of the Hamiltonian constraint is crucial for this result, so that demanding a non-singular evolution in quantum cosmology fixes the factor ordering ambiguity of the constraint: the scenario derived in this paper is possible with only one ordering, which belongs to the three standard choices (one could still choose different orderings of the extrinsic curvature operator entering the Lorentzian constraint, but since it is an observable in the kinematical sector it should be ordered symmetrically as done here).

Close to the classical singularity the discrete structure of space and time in quantum geometry is important which leads to large deviations from standard quantum cosmology [10]. This framework arises here as an approximation which is good only at large volume where the discrete volume spectrum is washed out to a continuous spectrum by inaccuracies. However, the exact description of loop quantum cosmology is also necessary to fix a unique solution which can be seen in the explicit solution corresponding to Euclidean four-space. For cosmological models with matter there is still a unique solution with appropriate semiclassical behavior: initial conditions are not imposed *ad hoc* but instead *derived* from the dynamical laws [31]. Taking into account the discreteness of the spectrum one can derive perturbative corrections for an effective Hamiltonian of standard quantum cosmology, but the completely non-perturbative description with discrete time is needed in order to study the fate of the classical singularity.

As an intuitive picture of the evolution of a universe in loop quantum cosmology we obtain the following one: starting in a semiclassical contracting state, it reaches a degenerate stage seen as the singularity in classical cosmology, in which the universe bounces off in order to enter an expanding branch. The further fate, whether it expands forever or recollapses in order to start a new such process, depends on the matter content and the value of the cosmological constant.

Appendices

A Euclidean Space in Standard Quantum Cosmology

Here we present classical and standard quantum cosmology of flat Euclidean space. For $\Gamma = 0$ the constraint equation (13) becomes $H^{(E)} = -6\kappa^{-1}c^2 \text{sgn}(p)\sqrt{|p|} = 0$ having two solutions $p = 0$ or $c = 0$. The first one only appears in a triad formulation and is of no physical interest because space is completely degenerate. Using (15) one can see that the second solution requires the extrinsic curvature to vanish, whereas it leaves the metric arbitrary, and thus gives flat Euclidean space (the metric does not change in coordinate time because of $\{p, H^{(E)}\} \approx 0$ on the constraint surface).

Standard quantum cosmology proceeds as follows: Using a factor ordering in which the metric variables appear on the right (this is the ordering resulting from loop quantum cosmology) solutions in the c -representation are such that a quantization of $\text{sgn}(p)\sqrt{|p|}$ acting on the wave function yields either $\delta(c)$ or $\delta'(c)$ due to the factor c^2 . There are some problems already in this simple model: First, $\text{sgn}(p)\sqrt{|p|}$ cannot be quantized to an invertible operator when the range of p contains the value zero, and a procedure like that leading to a bounded inverse scale factor in loop quantum cosmology is not available in standard quantum cosmology. Although Euclidean space does not contain a singularity, the point $p = 0$ leads to problems in the quantization. Second, there are two independent solutions only one of which, $\delta(c)$, corresponds to the classical solution; and there is no independent argument to exclude the other solution without referring explicitly to the classical situation. Both problems are solved in loop quantum cosmology, which is intimately related to the fate of the classical singularity.

B Hamiltonian Constraint for Models with Positive Spatial Curvature

For the isotropic, spatially positively curved model we need to take into account the holonomy $h_{[I,J]}$ in (18) which is h_K if ϵ_{IJK} is positive and h_K^{-1} if ϵ_{IJK} is negative. With this we have for isotropic holonomies

$$\begin{aligned} \sum_{IJK} \epsilon^{IJK} \text{tr} \left(h_I h_J h_I^{-1} h_J^{-1} h_{[I,J]}^{-1} h_K [h_K^{-1}, \hat{V}] \right) &= 3 \text{tr} \left(h_1 h_2 h_1^{-1} h_2^{-1} [h_3^{-1}, \hat{V}] \right) \\ &\quad - 3 \text{tr} \left(h_2 h_1 h_2^{-1} h_1^{-1} h_3^2 [h_3^{-1}, \hat{V}] \right) \end{aligned}$$

which yields

$$\begin{aligned} \hat{H}_+^{(E)} &= -48i(\gamma\kappa l_P^2)^{-1} \left(\sin(\tfrac{1}{2}c) - 2\sin^5(\tfrac{1}{2}c) - 2\sin^2(\tfrac{1}{2}c)\cos^3(\tfrac{1}{2}c) \right) \\ &\quad \times \left(\sin(\tfrac{1}{2}c)\hat{V}\cos(\tfrac{1}{2}c) - \cos(\tfrac{1}{2}c)\hat{V}\sin(\tfrac{1}{2}c) \right) \end{aligned}$$

with action

$$\begin{aligned}\hat{H}_+^{(\text{E})}|n\rangle &= 3(\gamma\kappa l_{\text{P}}^2)^{-1} \text{sgn}(n) \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) \left(\frac{1}{2}(1+i)|n+5\rangle + \frac{1}{2}(1-5i)|n+3\rangle \right. \\ &\quad \left. - (1-i)|n+1\rangle - (1+i)|n-1\rangle + \frac{1}{2}(1+5i)|n-3\rangle + \frac{1}{2}(1-i)|n-5\rangle \right) .\end{aligned}$$

From this we obtain the extrinsic curvature operator

$$\hat{K}_+|n\rangle = \frac{1}{8}l_{\text{P}}^2 \sum_{q=-5; q \text{ odd}}^5 K_{+,n}^{(-q)}|n+q\rangle$$

with

$$\begin{aligned}K_{+,n}^{(\pm 1)} &= \mp 6(1 \mp i)(\gamma l_{\text{P}}^2)^{-3} \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) \left(V_{\frac{1}{2}(|n \mp 1|-1)} - V_{\frac{1}{2}(|n|-1)} \right) \\ K_{+,n}^{(\pm 3)} &= \pm 6(5 \mp i)(\gamma l_{\text{P}}^2)^{-3} \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) \left(V_{\frac{1}{2}(|n \mp 3|-1)} - V_{\frac{1}{2}(|n|-1)} \right) \\ K_{+,n}^{(\pm 5)} &= \mp 6(1 \pm i)(\gamma l_{\text{P}}^2)^{-3} \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) \left(V_{\frac{1}{2}(|n \mp 5|-1)} - V_{\frac{1}{2}(|n|-1)} \right) .\end{aligned}$$

This leads to

$$\left(\sin(\tfrac{1}{2}c)\hat{K}_+ \cos(\tfrac{1}{2}c) - \cos(\tfrac{1}{2}c)\hat{K}_+ \sin(\tfrac{1}{2}c) \right) |n\rangle = \frac{1}{8}il_{\text{P}}^2 \sum_{q=-5; q \text{ odd}}^5 k_{+,n}^{(-q)}|n+q\rangle$$

with

$$k_{+,n}^{(q)} = \frac{1}{2}(K_{+,n+1}^{(q)} - K_{+,n-1}^{(q)})$$

which is non-zero for all n and q ($K_{+,n}^{(q)}$ is zero if and only if $n = 0$).

Taken together, this yields

$$\hat{P}_+|n\rangle = -\frac{3}{4}(1 + \gamma^{-2})(\gamma\kappa l_{\text{P}}^2)^{-1} \text{sgn}(n) \left(V_{\frac{1}{2}|n|} - V_{\frac{1}{2}|n|-1} \right) \sum_{k=-5}^5 A_n^{(-2k)}|n+2k\rangle$$

with

$$A_n^{(l)} := \sum_{q+r=l; -5 \leq q, r \leq 5; q, r \text{ odd}} k_{+,n}^{(q)} k_{+,n-q}^{(r)} .$$

Acknowledgements

The author is grateful to A. Ashtekar for suggestions, discussions, and a careful reading of the manuscript. This work was supported in part by NSF grant PHY00-90091 and the Eberly research funds of Penn State.

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