Inverse scale factor in isotropic quantum geometry

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The inverse scale factor, which in classical cosmological models diverges at the singularity, is quantized in isotropic models of loop quantum cosmology by using techniques which have been developed in quantum geometry for a quantization of general relativity. This procedure results in a *bounded* operator which is diagonalizable simultaneously with the volume operator and whose eigenvalues are determined explicitly. For large scale factors (in fact, up to a scale factor slightly above the Planck length) the eigenvalues are close to the classical expectation, whereas below the Planck length there are large deviations leading to a nondiverging behavior of the inverse scale factor even though the scale factor has vanishing eigenvalues. This is a first indication that the classical singularity is better behaved in loop quantum cosmology.

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I. INTRODUCTION

General relativity predicts singularities in many situations of astrophysical or cosmological interest, which means that there are limits for the classical theory beyond which it is no longer valid. A widespread expectation is that a quantization of gravity is inevitable in order to describe these regimes meaningfully, but up to now there has been no complete, generally accepted quantization of general relativity. For a long time, mini-superspace models obtained by a symmetry reduction of the classical theory with a subsequent quantization [1,2] (henceforth called ''standard quantum cosmology'' in the context of cosmological models) were the only approach to address those issues; but in view of the fact that the quantization techniques were those of simple quantum mechanical systems, which cannot be applied to the full theory, the results are not likely to hold true in a full quantization. In fact, it has been shown in quantum geometry [3] that geometry has a discrete structure leading, e.g., to a discrete volume spectrum [4,5], whereas in standard quantum cosmology the scale factor, and so the volume, is still continuous with a range from zero to infinity. For large volume, this is a very good approximation to the discrete volume spectrum of quantum geometry, but just in the domain close to the classical singularity there are huge deviations between the discrete and the continuous spectra.

Therefore, we follow a different approach to quantum cosmology which has been initiated in [6–11] and which starts by selecting symmetric (isotropic, and in particular homogeneous, in this paper) states in the kinematical Hilbert space of quantum geometry. This means that the symmetry reduction is not purely classical, but is done after an essential step of the quantization which already leads to the discrete structure of space. Consequently, the volume spectrum of cosmological models is discrete and even known explicitly in the isotropic case [8]. The simplification of the spectrum caused by symmetry (interpreted analogously to the familiar level splitting in the spectroscopy of atoms) is very fortunate because it facilitates explicit calculations. Reciprocally, the discreteness of the volume spectrum implies that the models of loop quantum cosmology embody the distinctive feature of quantum geometry of having a discrete structure. In fact, the quantization techniques of loop quantum cosmology are designed to be as close to those of the full theory as possible, with only slight adaptations to the symmetry. So those models can be used for crucial tests of methods developed in the full theory, but they have also been used to derive new properties, e.g., a discrete time and discrete physical (not just kinematical) spectra of geometric operators [10].

In this paper we will use techniques which have been developed in order to quantize the Hamiltonian constraint and matter Hamiltonians in the full theory [12,13] for a quantization of the inverse scale factor in isotropic quantum geometry. As a result we will derive a bounded operator despite the fact that the volume or the scale factor has vanishing eigenvalues. The underlying ''mechanism'' is the same as the one which ensures, in the full theory, that matter Hamiltonians can be quantized to obtain densely defined operators. One might suspect that this is simply a mathematical trick which serves to remove singularities but which will spoil the classical limit. We will show that this is not the case: singularities are removed, but the classical regime is not affected. In fact, for the inverse scale factor the classical theory turns out to be an excellent approximation right up to a scale factor of the order of the Planck length. This is quite unexpected; *a priori*, one expects the classical behavior to be valid only for scale factors very large compared to the Planck length.

The plan of the paper is as follows. First, we will recall the framework of isotropic loop quantum cosmology and extend the methods developed in [8] to gauge non-invariant states in Sec. II. This will then be applied for a discussion of the inverse scale factor which is quantized in Sec. III. We will determine all its eigenstates and its complete spectrum and study the two interesting regimes for very small and large scale factors. In the final section we will present our conclusions concerning the validity of quantization techniques and the quantum picture of the classical singularity.

II. ISOTROPIC QUANTUM GEOMETRY

The general framework for a symmetry reduction of quantized diffeomorphism invariant theories has been developed

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in [6] and specialized to homogeneous and isotropic models in [7]. Symmetric states are defined at the kinematical level of the quantum theory, and thus have properties very different from those of states obtained after quantizing a classically reduced theory. Still, for explicit expressions of symmetric states and operators we need to know the symmetry reduction of a theory of connections and triads which we will sketch first in the case of isotropy.

Isotropic connections are of the form $A_a^i=\phi_I^i\omega_a^I=c\Lambda_I^i\omega_a^I$, where $\Lambda_I=\Lambda_I^i\tau_i$ is an internal $SU(2)$-dreibein (which is purely a gauge choice) and ω^I are left-invariant one-forms on the ''translational part'' N of the symmetry group $S\cong N\rtimes SO(3)$ acting on the space manifold Σ. [Here, $\tau_j=-(i/2)\sigma_j$ are generators of $SU(2)$ with σ_j the Pauli matrices; N is isomorphic to $\mathbb{R}^3$ for the spatially flat model or $SU(2)$ for the spatially positively curved model.] For homogeneous models, the nine parameters ϕ_I^i are arbitrary. A cotriad can be expressed as $e_a^i=a_I^i\omega_a^I=a\Lambda_I^i\omega_a^I$ with the scale factor[1] $|a|$. 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[2] $E_i^a=p_i^IX_I^a=p\Lambda_i^IX_I^a$ where $p=\mathrm{sgn}(a)a^2$. In addition to gauge freedom, there are only the two canonically conjugate variables c and p which embody the gauge invariant information of the connection and triad. Information about the geometry of space is fully contained in p, which is the square of the radius of a spacelike slice. The Liouville form

$$(\gamma\kappa)^{-1}p_i^I\mathrm{d}\phi_I^i=(\gamma\kappa)^{-1}p\mathrm{d}c\Lambda_i^I\Lambda_I^i=3(\gamma\kappa)^{-1}p\mathrm{d}c$$

leads to the symplectic structure

$$\{c,p\}=\tfrac{1}{3}\gamma\kappa \tag{1}$$

($\kappa=8\pi G$ is the gravitational constant and γ the Barbero-Immirzi parameter). The factor $\frac{1}{3}$ has been overlooked in [8], and so also the derivative operators and the volume spectrum derived there have to be corrected by appropriate factors. We will do this in the formulas below.

Isotropic states in the connection representation are defined as distributional states in the full theory which are supported only on isotropic connections. Since all the information of an isotropic connection is contained in one $SU(2)$-element [$\exp(c\Lambda_3^i\tau_i)$, say] the reduced kinematical Hilbert space can be taken to be the space $\mathcal{H}_{\mathrm{kin}}=L^2(SU(2),\mathrm{d}\mu_H)$ of square integrable functions on $SU(2)$ with respect to the Haar measure. However, gauge invariance is not imposed in the obvious sense by conjugation on this copy of $SU(2)$, but instead in such a way that there is a larger class of gauge invariant functions (see [8] for details). In addition to the usual character functions

$$\chi_j=\frac{\sin(j+\frac{1}{2})c}{\sin\frac{1}{2}c}, \tag{2}$$

where j is a non-negative half-integer, we have gauge-invariant states given by $\zeta_{-1/2}=(\sqrt{2}\sin\frac{1}{2}c)^{-1}$ and

$$\zeta_j=\frac{\cos(j+\frac{1}{2})c}{\sin\frac{1}{2}c}. \tag{3}$$

All states (χ_j,ζ_j) form an orthonormal basis of the gauge invariant kinematical Hilbert space. The fact that we need the functions ζ_j and also the value $j=-\frac{1}{2}$ can be seen from a representation of the kinematical Hilbert space as periodic functions in c, where the measure provides a factor $\sin^2\frac{1}{2}c$. A complete set of those functions is given by sin and cos with the above frequencies. Gauge noninvariant functions are given by $\Lambda_I^i\chi_j$ and $\Lambda_I^i\zeta_j$ where Λ_I^i is the internal dreibein and provides pure gauge degrees of freedom.

In [8] the volume operator $\hat{V}$ has been shown to have the eigenstates χ_j, ζ_j with eigenvalues (corrected here for the missing factor $\frac{1}{3}$ in the symplectic structure and derivative operators)

$$V_j=(\gamma l_{\mathrm{P}}^2)^{3/2}\sqrt{\tfrac{1}{27}j(j+\tfrac{1}{2})(j+1)}. \tag{4}$$

The eigenvalue zero is three-fold degenerate, whereas all other eigenvalues are positive and twice degenerate. The two-fold degeneracy arises naturally in a triad formulation because any value of the volume can be achieved in two different orientations of the triad. Intuitively, this demonstrates the necessity of the states ζ_j besides the characters χ_j. Taking the cubic root yields the eigenvalues of the scale factor $|a|$ which are shown in Fig. 1.

However, in [8] the action of $\hat{V}$ has not been determined on gauge noninvariant states. An extension to those states is done by using gauge invariance of the volume, which implies $[\Lambda_I^i,\hat{V}]=\alpha\Lambda_I^i$ for some $\alpha\in\mathbb{R}$. We can now use $\Sigma_i\Lambda_I^i\Lambda_i^I=1$ (no sum over I) in order to obtain

$$0=\left[\sum_i\Lambda_I^i\Lambda_i^I,\hat{V}\right]=\sum_i\Lambda_I^i[\Lambda_i^I,\hat{V}]+\sum_i[\Lambda_I^i,\hat{V}]\Lambda_i^I=2\alpha$$

and so $\alpha=0$. Thus, the volume operator commutes with Λ_I^i (acting as a multiplication operator in the connection representation) and we can trivially extend its action to gauge noninvariant states.

All we need for the following calculations is the action of $\cos\frac{1}{2}c$ and $\sin\frac{1}{2}c$ appearing in the ''point holonomy'' [14] h_I

[1] In a triad formulation we use a variable a which can take both signs, even though the two sectors of positive and negative a, respectively, are disconnected in a metric formulation.

[2] Note that, in contrast to [7], we use the physical metric in order to provide the density weight and not an auxiliary homogeneous metric: $p_i^I:=|\det a_j^j|a_i^I$, a_i^I being inverse to a_I^i. Nevertheless, we need to fix a reference system already in order to define the action of our symmetry group, which leads to the factor of V_0 in the formulas of [7,8]. However, this factor is an artifact of the homogeneous models and not of physical significance. It just tells us that we cannot define an absolute scale factor in a diffeomorphism invariant setting, but only a relative one with respect to some given value. In this paper we will set $V_0=1$.

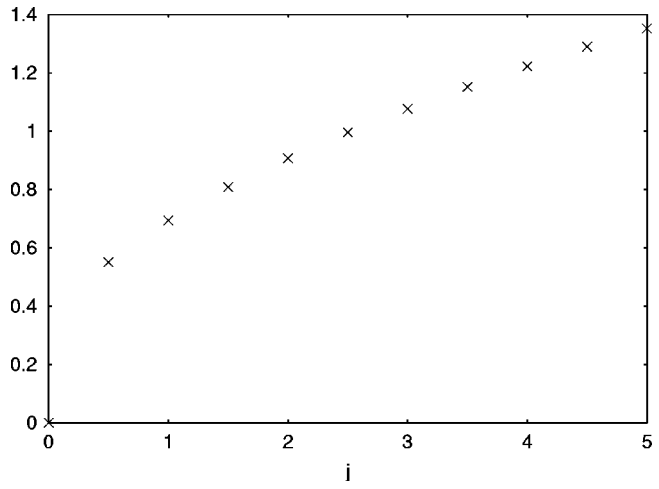

FIG. 1. Eigenvalues $V_j^{1/3}$ of the scale factor (in units of $\sqrt{\gamma}l_{\rm P}$).

$:=\exp(c\Lambda_I^i\tau_i)=\cos(\frac{1}{2}c)+2\sin(\frac{1}{2}c)\Lambda_I^i\tau_i$ which in quantum geometry serves as the basic multiplication operator. This can be obtained in the connection representation (2),(3) by using trigonometric relations leading for $j\geqslant\frac{1}{2}$ to

$$\cos(\tfrac{1}{2}c)\chi_j=\tfrac{1}{2}(\chi_{j+1/2}+\chi_{j-1/2}),$$

$$\cos(\tfrac{1}{2}c)\zeta_j=\tfrac{1}{2}(\zeta_{j+1/2}+\zeta_{j-1/2}) \tag{5}$$

$$\sin(\tfrac{1}{2}c)\chi_j=-\tfrac{1}{2}(\zeta_{j+1/2}-\zeta_{j-1/2}),$$

$$\sin(\tfrac{1}{2}c)\zeta_j=\tfrac{1}{2}(\chi_{j+1/2}-\chi_{j-1/2}) \tag{6}$$

with certain modifications in numerical coefficients for $j=0$ or $j=-\frac{1}{2}$, which are not important for our purposes.

Because of the exceptional formulas for low j it is more convenient to use the states

$$|n\rangle:=\frac{\exp(\frac{1}{2}inc)}{\sqrt{2}\sin\frac{1}{2}c},\quad n\in\mathbb{Z} \tag{7}$$

which are decomposed in the previous states by

$$|n\rangle=2^{-1/2}(\zeta_{1/2(|n|-1)}+i\,\mathrm{sgn}(n)\chi_{1/2(|n|-1)})$$

for $n\neq 0$ and $|0\rangle=\zeta_{-1/2}$. The label n of a state $|n\rangle$ is proportional to the eigenvalue of the dreibein operator [8] [note the factor $\frac{1}{3}$ in order to correct for the symplectic structure (1)]

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

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

$$\cos(\tfrac{1}{2}c)|n\rangle=\tfrac{1}{2}(|n+1\rangle+|n-1\rangle),$$

$$\sin(\tfrac{1}{2}c)|n\rangle=-\tfrac{1}{2}i(|n+1\rangle-|n-1\rangle)$$

for all integer n.

III. QUANTIZATION OF THE INVERSE SCALE FACTOR

In isotropic geometries, the classical singularity is signaled by the inverse scale factor $|a|^{-1}$ which diverges for $a=0$ and occurs by some positive power in all diverging curvature components. Classically, we have $|a|^{-1}=V^{-1/3}$ so that one might try to quantize it by using the inverse volume operator. This inverse, however fails to be a densely defined operator because $\hat{V}$ has the eigenvalue zero (with threefold degeneracy: $\hat{V}$ annihilates $\zeta_{-1/2}$, χ_0 and ζ_0). Thus, we have to look for another approach. We will use an expression which classically reduces to the inverse scale factor but is better suited for a quantization, namely

$$m_{IJ}:=\frac{q_{IJ}}{\sqrt{\det q}}=\frac{a_I^i a_I^i}{|\det(a_I^i)|}=\frac{1}{|a|}\,\delta_{IJ} \tag{8}$$

in terms of the isotropic metric $q_{IJ}=a^2\delta_{IJ}$ or the triad components a_I^i. Since the latter are not fundamental variables, one needs a prescription to quantize them. Here one can make use of the classical identity

$$e_a^i=2(\gamma\kappa)^{-1}\{A_a^i,V\} \tag{9}$$

and quantize the co-triad by expressing the connection in terms of a holonomy, using the volume operator and turning the Poisson bracket into a commutator. This method has been successfully employed in [12] in order to quantize the Hamiltonian constraint of the full theory. In this section we carry out a similar procedure for a quantization of the inverse scale factor. The regularization scheme adapted to isotropic models is reviewed in Sec. III A and then applied to m_{IJ} in Sec. III B where we derive an operator $\hat{m}_{IJ}$. Its spectrum is determined in Sec. III C followed by a discussion of its main features and viability (Sec. III D).

A. The regularization scheme

Let us first recall from [9] the regularization scheme. As noted in [12], it is important to be aware of the density weight when regularizing expressions in a diffeomorphism invariant field theory: only scalar quantities, usually space integrals of weight 1 densities, can be quantized in a background independent manner. This is also important in our reduced models. Although we do not have the freedom to make arbitrary coordinate transformations since most of them would violate the symmetry conditions, we do have dilatations with a scale parameter ϵ which allow us to keep track of the density weight. These scale transformations also play an important role in adapting the regularization of [12] in the full theory to reduced models (see [9] for details). We will proceed along the lines of the following recipe: Starting from a classical expression in the full theory we first insert homogeneous fields parametrized by the components ϕ_I^i, p_i^I, . . . and arrive at the reduced expression for a homogeneous model. Now we start the regularization by performing a scale transformation with parameter ϵ. Taking care

of the density weights, we have to multiply any one-form component by ϵ, any density-weighted vector field component by ϵ^2, Poisson brackets by ϵ^{-3}, etc. Our original expression, a density integrated over space, then gets multiplied by a factor ϵ^3 which is absorbed in the rescaled space volume. In a homogeneous model, the continuum limit needed in the regularization is replaced by a limit $\epsilon\to 0$ which means, e.g., that connection components ϕ^i_I can be approximated by holonomies $h_I=\exp(\epsilon\phi^i_I\tau_i)=1+\epsilon\phi^i_I\tau_i+O(\epsilon^2)$ as in the full theory. The quantized expression, on the other hand, will be independent of ϵ; for a detailed discussion see [9].

If we are interested in isotropic models, we have to perform another step because the homogeneous coefficients have to be put in isotropic form thereby yielding the isotropic classical expressions. In the quantization, we also start from the quantized homogeneous operator and insert special holonomies $h_I=\cos(\frac{1}{2}c)+2\sin(\frac{1}{2}c)\Lambda^i_I\tau_i$ which leads to the operators $\cos\frac{1}{2}c$ and $\sin\frac{1}{2}c$ whose action we already know. Derivative operators are treated similarly, but we usually only need the volume operator which has already been derived [8].

We illustrate a typical calculation by computing the Poisson brackets

$$\{\sin\tfrac{1}{2}c,V\}=\{\sin\tfrac{1}{2}c,|p|^{3/2}\}=\tfrac{1}{4}\gamma\kappa\cos(\tfrac{1}{2}c)\sqrt{|p|}\,\mathrm{sgn}(p)$$

using the symplectic structure (1). The corresponding commutator of the quantized objects acts on χ_j as

$$[\sin\tfrac{1}{2}c,\hat{V}]\chi_j=\tfrac{1}{2}(V_{j+1/2}-V_j)\zeta_{j+1/2}+\tfrac{1}{2}(V_j-V_{j-1/2})\zeta_{j-1/2}$$

$$\sim\frac{1}{4\sqrt{3}}(\gamma l_{\mathrm{P}}^2)^{3/2}\sqrt{j}\cdot\tfrac{1}{2}(\zeta_{j+1/2}+\zeta_{j-1/2})$$

which we expanded in the last line for large j. A quantization of $\sqrt{|p|}\,\mathrm{sgn}(p)$ should have the asymptotic behavior $\chi_j\mapsto i\sqrt{\gamma l_{\mathrm{P}}^2}\sqrt{j/3}\zeta_j$ for large j (because of the sign it maps χ to $i\zeta$ and vice versa, and the factor $\sqrt{j/3}$ follows from the large-j behavior of the volume spectrum). So we see that for large j (where the ordering is irrelevant) the commutator is $\frac{1}{4}i\gamma l_{\mathrm{P}}^2\cos(\frac{1}{2}c)\sqrt{|\hat{p}|}\,\mathrm{sgn}(\hat{p})$ which demonstrates that we have the correct expression corresponding to $i\hbar$ times the classical Poisson brackets. For the correct prefactor $\frac{1}{4}$ it is important that we used the symplectic structure (1) and corrected the volume eigenvalues.

B. Quantization

In order to quantize the inverse scale factor we use the expression (8). However, it is not a density and thus for a regularization along the above lines we need to first transform it into an expression which is a density such that it can be integrated to a scalar. This can easily be achieved by contracting with two density weighted vector fields, e.g. the electric field E^a, leading to the electric part of the Maxwell Hamiltonian

$$H=\int\mathrm{d}^3x\frac{q_{ab}}{\sqrt{\det q}}E^aE^b.$$

In this paper we are only interested in the gravitational part which will be separated later, but the full expression can be used for studying, e.g., Maxwell theory coupled to quantum gravity.

First we have to insert homogeneous co-triad components $e^i_a=a^i_I\omega^I_a$ and also homogeneous electric fields $E^a=E^IX^a_I$ (we also integrate over space and suppress the resulting factor of the coordinate volume setting $V_0=1$):

$$H=\frac{a^i_Ia^i_J}{\sqrt{|\det(p^I_i)|}}E^IE^J.$$

Now we have to express the co-triad components a^i_I by Poisson brackets using Eq. (9). This expression can be derived by first computing

$$\begin{aligned}\{\phi^k_K,\epsilon_{MNL}\epsilon^{ijl}p^M_ip^N_jp^L_l\}&=3\gamma\kappa\epsilon^{ijk}\epsilon_{MNK}p^M_ip^N_j\\&=3\gamma\kappa\epsilon^{ijk}\epsilon_{ijl}a^l_K\mathrm{sgn}(\det(p^M_m))\\&\quad\times\sqrt{|\det(p^M_m)|}\\&=6\gamma\kappa a^k_K\mathrm{sgn}(\det(p^M_m))\\&\quad\times\sqrt{|\det(p^M_m)|}\end{aligned}$$

where we have used $\delta^L_K=p^L_ia^l_K|\det p^M_m|^{-1/2}$ in the second step. We thus have the reduction of Thiemann's identity [12] to homogeneous variables:

$$\begin{aligned}a^k_K&=[\gamma\kappa\mathrm{sgn}(\det(p^M_m))]\sqrt{|\det(p^M_m)|})^{-1}\{\phi^k_K,\det(p^M_m)\}\\&=2(\gamma\kappa)^{-1}\{\phi^k_K,\sqrt{|\det(p^M_m)|}\}\\&=2(\gamma\kappa)^{-1}\{\phi^k_K,V\}.\end{aligned}\tag{10}$$

We insert this expression in H to obtain

$$H=4(\gamma\kappa)^{-2}\frac{\{\phi^i_I,V\}\{\phi^i_J,V\}}{V}E^IE^J=16(\gamma\kappa)^{-2}\{\phi^i_I,\sqrt{V}\}\times\{\phi^i_J,\sqrt{V}\}E^IE^J$$

which we now use for the regularization. Note that we were able to absorb the V in the denominator into the Poisson bracket in the numerator, as first done in [12]. *This is the key point leading to a bounded operator after quantization.*

We now multiply the components ϕ^i_I, E^I, the volume and the Poisson brackets by the factors ϵ, ϵ^2, ϵ^3 and ϵ^{-3}, respectively, and obtain the regularized expression (absorbing ϵ^{-3} in the space integral)

$$\begin{aligned}H_\epsilon&=16(\gamma\kappa)^{-2}\{\epsilon\phi^i_I,\sqrt{V}\}\{\epsilon\phi^i_J,\sqrt{V}\}\epsilon^2E^I\epsilon^2E^J\\&=-32(\gamma\kappa)^{-2}\mathrm{tr}(h_I\{h_I^{-1},\sqrt{V}\}h_J\{h_J^{-1},\sqrt{V}\})\\&\quad\times\epsilon^2E^I\epsilon^2E^J+O(\epsilon^7).\end{aligned}$$

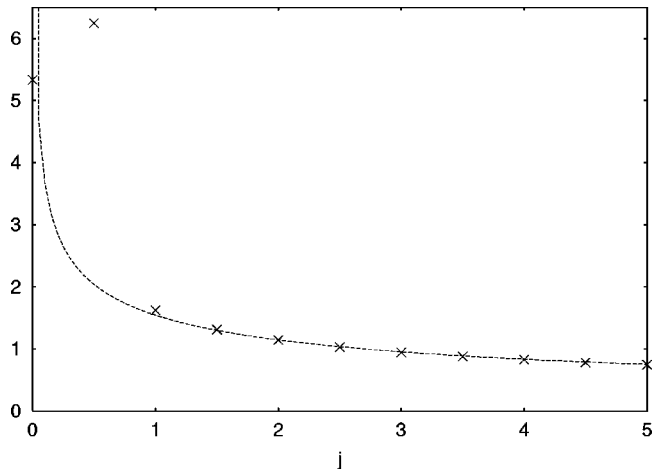

FIG. 2. Eigenvalues $m_{II,j}$, $j \geq 0$ [in units of $(\gamma l_{\mathrm{P}}^2)^{-1/2}$] of the inverse scale factor ($\times$) compared to the classical expectation $V_j^{-1/3}$ (dashed line).

Now we can read off the gravitational part and immediately quantize: The remaining factors of ϵ^2 are needed for a quantization of the electric field components, whereas the rest yields

$$\hat{m}_{IJ} = 32(\gamma l_{\mathrm{P}}^2)^{-2} \mathrm{tr}(h_I[h_I^{-1}, \sqrt{\hat{V}}] h_J[h_J^{-1}, \sqrt{\hat{V}}]) \qquad (11)$$

which is independent of the regulator ϵ.

So far, we have only used homogeneity; next, we can reduce Eq. (11) to isotropy: We have to insert the special form of holonomies and the isotropic volume operator and can then take the trace over the dreibein components Λ_I to arrive at the isotropic inverse scale factor

$$\begin{aligned}\hat{m}_{IJ} = 64(\gamma l_{\mathrm{P}}^2)^{-2} \{ & [\sqrt{\hat{V}} - \cos(\tfrac{1}{2}c)\sqrt{\hat{V}}\cos(\tfrac{1}{2}c) \\ & - \sin(\tfrac{1}{2}c)\sqrt{\hat{V}}\sin(\tfrac{1}{2}c)]^2 - \delta_{IJ}[\sin(\tfrac{1}{2}c)\sqrt{\hat{V}}\cos(\tfrac{1}{2}c) \\ & - \cos(\tfrac{1}{2}c)\sqrt{\hat{V}}\sin(\tfrac{1}{2}c)]^2\}. \end{aligned} \qquad (12)$$

This operator has two striking features. First, it provides a quantization of the inverse scale factor by a *bounded operator* despite the fact that the classical expression diverges for $a \to 0$. As seen in Fig. 2, the upper bound is given by its eigenvalue in the state with $j = \frac{1}{2}$ and has the value $\frac{32}{3}(2 - \sqrt{2})(\gamma l_{\mathrm{P}}^2)^{-1/2}$ which diverges for $\hbar \to 0$. Thus it is the finiteness of Planck's constant that removes the infinity of the classical inverse scale factor. This is somewhat analogous to the ground state energy of the hydrogen atom: it is negative and finite in quantum theory, but diverges for $\hbar \to 0$ in correspondence with the fact that the classical energy is unbounded from below. The second feature is that the operator-valued matrix $\hat{m}_{IJ}$ is not diagonal as in the classical case. As one would expect, the off-diagonal components have a purely quantum origin and go to zero as $\hbar$ tends to zero. In order to critically examine the viability of the quantization procedure we need to discuss the classical limit which we will do below after deriving the complete spectrum of $\hat{m}_{IJ}$.

C. Spectrum of the inverse scale factor

Both squared brackets in the operator (12) act diagonally on the states χ_j, ζ_j which can be derived by using the volume eigenvalues (4) and the operators $\cos\frac{1}{2}c$ and $\sin\frac{1}{2}c$ in Eqs. (5), (6). The result is

$$\begin{aligned}[\sqrt{\hat{V}} - \cos(\tfrac{1}{2}c)\sqrt{\hat{V}}\cos(\tfrac{1}{2}c) - \sin(\tfrac{1}{2}c)\sqrt{\hat{V}}\sin(\tfrac{1}{2}c)]^2\chi_j \\ = (\sqrt{V_j} - \tfrac{1}{2}\sqrt{V_{j+1/2}} - \tfrac{1}{2}\sqrt{V_{j-1/2}})^2\chi_j \\ [\sin(\tfrac{1}{2}c)\sqrt{\hat{V}}\cos(\tfrac{1}{2}c) - \cos(\tfrac{1}{2}c)\sqrt{\hat{V}}\sin(\tfrac{1}{2}c)]^2\chi_j \\ = -\tfrac{1}{4}(\sqrt{V_{j+1/2}} - \sqrt{V_{j-1/2}})^2\chi_j \end{aligned}$$

and analogously on ζ_j (the state $\zeta_{-1/2}$ is annihilated by both operators, so we have to define $V_{-1} = 0$ when using the above formulas in this case).

Inserting these operators in Eq. (12) we immediately obtain the eigenvalues

$$\begin{aligned} m_{IJ,j} = 16(\gamma l_{\mathrm{P}}^2)^{-2} [& \delta_{IJ}(\sqrt{V_{j+1/2}} - \sqrt{V_{j-1/2}})^2 + 4(\sqrt{V_j} \\ & - \tfrac{1}{2}\sqrt{V_{j+1/2}} - \tfrac{1}{2}\sqrt{V_{j-1/2}})^2] \end{aligned} \qquad (13)$$

in terms of the volume eigenvalues. Note that there are also nonvanishing off-diagonal terms which are independent of I, J. Using Eq. (4) we can expand the eigenvalues of the product $\hat{V}^{1/3}\hat{m}_{IJ}$, which classically should be δ_{IJ}:

$$\begin{aligned} m_{IJ,j} &= V_j^{-1/3}[\delta_{IJ} + (\tfrac{1}{256} + \tfrac{37}{192}\delta_{IJ})j^{-2} + O(j^{-3})] \\ &\sim V^{-1/3}[\delta_{IJ} + \tfrac{1}{9}(\tfrac{1}{256} + \tfrac{37}{192}\delta_{IJ})\gamma^2 l_{\mathrm{P}}^4 a^{-4}]. \end{aligned} \qquad (14)$$

For large j we used the approximation $a^2 = |p| \sim \frac{1}{3}\gamma l_{\mathrm{P}}^2 j$. This demonstrates that the leading order is in fact given by $V^{-1/3}\delta_{IJ}$ and higher order corrections only start with $l_{\mathrm{P}}^4 a^{-4}$. Also the *off-diagonal terms*, which are of purely quantum origin, *only arise at this order*. Thus, we have the correct behavior in the classical regime of a large scale factor (since the only way to obtain dimensionful geometric quantities is by multiplying a given function of j by l_{P}, the classical limit with $l_{\mathrm{P}} \to 0$ also involves $j \to \infty$, as in the treatment of angular momentum in quantum mechanics) and we see that all the techniques involved in the quantization of the inverse scale factor are perfectly compatible with the classical limit. Note also that the leading order in the expansion is independent of the Barbero-Immirzi parameter γ.

In fact, the classical behavior can be observed in a range by far larger than expected from the j^{-1}-expansion. As can be seen in Figs. 2 and 3, even down to $j = 1$, i.e. for a scale factor slightly above the Planck length, the eigenvalues lie close to the classical expectation. Only the lowest eigenvalues deviate strongly from the classical curve, but this is in a regime where quantum effects are important. Those effects are responsible for the boundedness of the quantized inverse scale factor and its finite eigenvalues even on the states χ_0, ζ_0 and $\zeta_{-1/2}$ which are annihilated by the volume operator.

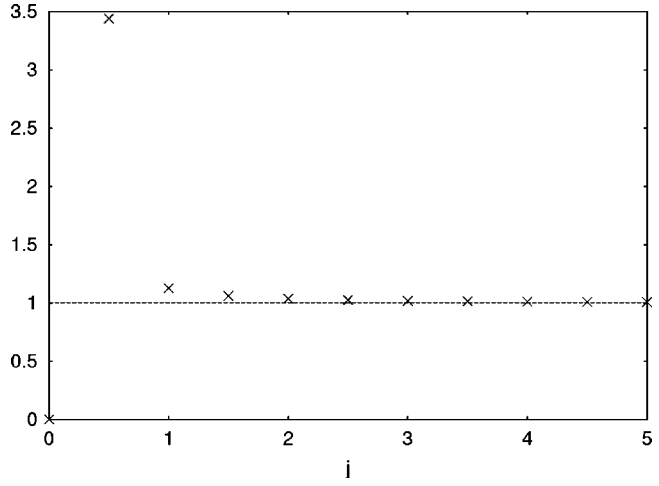

FIG. 3. Product $V_j^{1/3} m_{II,j}$ of eigenvalues of the scale factor and the inverse scale factor compared to the classical expectation one (dashed line).

As expected from the fact that both classical quantities only depend on the triad degrees of freedom, the volume operator $\hat{V}$ and the quantized inverse scale factor $\hat{m}_{IJ}$ are simultaneously diagonalizable. The surprising fact is that $\hat{m}_{IJ}$ is a densely defined operator with the correct classical behavior in a wide range. Thus, even in states which are annihilated by the volume operator we must have finite eigenvalues of $\hat{m}_{IJ}$; otherwise $\hat{m}_{IJ}$ would not be densely defined. Since $\hat{m}_{II}$ is a quantization of the inverse scale factor, such a behavior would be impossible in the classical description where we have the identity $V^{1/3} m_{IJ} = \delta_{IJ}$. In quantum theory, while this relation *is* valid at large volume (see Fig. 3), quantum corrections cause large deviations at the Planck scale close to the zero volume states. Thus, $\hat{V}$ and $\hat{m}_{II}$ are not inverse operators of each other, which in particular allows finite eigenvalues of $\hat{m}_{II}$ in states annihilated by $\hat{V}$. This is a new mechanism with the origin purely in quantum geometry by which the classical singularity is resolved.

D. The $j=-\frac{1}{2}$-state

Two aspects of the quantization of the inverse scale factor are important: first, it is a bounded operator cutting off the classical divergence and simultaneously preserving the classical behavior for values of the volume larger (not much larger) than a Planck cube. This fact is welcome and can be understood as originating in quantum effects which become important only for small volume where the classical theory breaks down. Technically, this is done by choosing an appropriate classical expression as the starting point for quantization. Since the volume operator has zero eigenvalues, its inverse does not exist and, therefore, cannot be used for a quantization of the inverse scale factor. But as we have seen, it is possible to rewrite the inverse scale factor as the expression (8) which is quantized to a bounded operator (12). In this way, it is understandable that the quantization $\hat{m}_{IJ}$ of the classical quantity $m_{IJ} = |a|^{-1} \delta_{IJ}$ does not coincide with the (nonexisting) inverse "$\hat{a}^{-1}$" of the quantization of a. Such effects are not unexpected in quantum theory. A second feature of the quantization of the inverse scale factor seems to be more questionable: one of the zero volume eigenstates has also a zero (not just finite) eigenvalue of the inverse scale factor and so both $\hat{a}$ and $\hat{m}_{II}$ annihilate the same state. Of course, this happens at a point where the classical theory completely breaks down and classical intuition cannot be trusted, but still an elucidation is needed.[3] This is even more important because these issues are essential for a quantum evolution through the classical singularity [15,16].

A basic observation in this respect is that the classical value of the inverse scale factor m_{IJ} corresponding to the quantization (11) is not defined at $a=0$, and so m_{IJ} has to be appropriately extended to this point. This can formally be done as $m_{IJ} := \mathrm{sgn}(a)^2 |a|^{-1} \delta_{IJ}$ (taking into account the derivative of $V = |p|^{3/2}$ in the Poisson bracket) which, of course, is the same as Eq. (8) on the classically allowed region $a>0$. In the point $a=0$ both this expression and a^{-1} are ill-defined and so its introduction does not change the classical situation. [The sign does not lead to a better behavior since it is, as the derivative of the absolute value, not well-defined for $a=0$; and even the standard definition $\mathrm{sgn}(0) := 0$ leads to an undefined expression "0/0," whereas the limit $a \to 0$ is not different from the one for a^{-1}.] However, as we have seen the situation is very different upon quantization which leads to a well-defined formulation also at states corresponding to the classical value $a=0$.

In order to illustrate this point, one can do essentially the same quantization in a simpler model which is the standard quantum theory of the cylinder T^*S^1 with canonically conjugate coordinates $\{\phi, \pi\} = 1$. Its states are $|n\rangle = \exp(in\phi)$ on which the basic operators act as

$$\cos\phi |n\rangle = \tfrac{1}{2}(|n+1\rangle + |n-1\rangle) \tag{15}$$

$$\sin\phi |n\rangle = -\tfrac{1}{2} i (|n+1\rangle - |n-1\rangle) \tag{16}$$

and

$$\hat{\pi} |n\rangle = n\hbar |n\rangle. \tag{17}$$

Being interested in a quantization of $|\pi|^{-1/2}$, one cannot use the inverse of $\hat{\pi}$, which does not exist. Instead, one can rewrite

$$\mathrm{sgn}(\pi) |\pi|^{-1/2} = 2(\cos\phi \{\sin\phi, \sqrt{|\pi|}\} - \sin\phi \{\cos\phi, \sqrt{|\pi|}\}) \tag{18}$$

which is a classical identity and clearly shows the origin of the sign. We used a similar identity (Thiemann's) to rewrite the inverse scale factor in isotropic cosmological models. It is also clear that one cannot use an analogous formula to rewrite $|\pi|^{-1/2}$ itself, since one always needs to take derivatives of the absolute value of π. But in $\pi=0$ both classical expressions are ill-defined and so there is no "correct" one

[3]The author is grateful to A. Ashtekar for raising this issue.

as a starting point for quantization. The only difference is that, as we will see shortly, $\mathrm{sgn}(\pi)|\pi|^{-1/2}$ can be quantized to a densely defined operator, whereas $|\pi|^{-1/2}$ cannot.

Expression (18) can easily be quantized by turning the Poisson brackets into $(i\hbar)^{-1}$ times commutators which leads to

$$\mathrm{sgn}(\hat{\pi})|\hat{\pi}|^{-1/2} = -2i\hbar^{-1}(\cos\phi[\sin\phi, \sqrt{|\hat{\pi}|}] - \sin\phi[\cos\phi, \sqrt{|\hat{\pi}|}]). \tag{19}$$

Using Eqs. (15), (16) and (17), its action on the states $|n\rangle$ can be computed which shows that $|n\rangle$ are eigenstates with eigenvalues

$$\sqrt{|n+1|\hbar^{-1}} - \sqrt{|n-1|\hbar^{-1}}. \tag{20}$$

For large $|n|$, one can perform a Taylor expansion demonstrating the correct classical limit

$$\begin{aligned}
&\sqrt{|n+1|\hbar^{-1}} - \sqrt{|n-1|\hbar^{-1}} \\
&\quad = \hbar^{-1/2}\sqrt{|n|}(\sqrt{1+n^{-1}} - \sqrt{1-n^{-1}}) \\
&\quad = \hbar^{-1/2}\sqrt{|n|}[n^{-1} + O(n^{-3})] \\
&\quad = \mathrm{sgn}(n)(|n|\hbar)^{-1/2} \\
&\qquad \times [1 + O(n^{-2})].
\end{aligned}$$

On the other hand, for $n=0$ the eigenvalue is zero, which is the same situation as in the quantization of the inverse scale factor: both $\hat{\pi}$ and $\mathrm{sgn}(\hat{\pi})|\hat{\pi}|^{-1/2}$ annihilate the same state. In view of the sign appearing with the inverse this is less surprising than initially, but again we emphasize that the sign makes no difference for the acceptability of the classical quantity. This toy example demonstrates that the important features of the quantization of the inverse scale factor are not special and can also be obtained in standard quantum mechanics. Nevertheless one may ask why such quantizations have not been used before. The answer is related to the classically allowed regions of the canonical coordinates, which are different in the T^*S^1-example and in isotropic cosmological models: on the cylinder, the full range for π is allowed including $\pi=0$ and so the inverse of π is not well-defined and also not of physical interest. But in the gravity model, the scale factor a must be positive classically, and so a^{-1} is well-defined on the classical phase space. In contrast to the inverse angular momentum π^{-1}, it is of direct physical interest since it appears, e.g., in curvatures.

IV. DISCUSSION

Isotropic cosmological models are not only interesting as models of an expanding universe, for which they have been widely used in the past century, but also provide systems in which explicit calculations are feasible, and therefore are excellent test arenas for sophisticated techniques developed for a quantization of general relativity. The basic technique used in this paper is the quantization of the co-triad components due to Thiemann [12]. Most of the operators studied so far in quantum geometry are built from the fundamental holonomies or derivative operators quantizing the triad components. The co-triad, however, is not a fundamental field in this framework, and so its quantization is less clear-cut. Nevertheless, it is of importance because it enters the quantization of the Hamiltonian constraint, which controls the dynamics of the theory. Models like the isotropic ones can be used to investigate quantization ambiguities in detail, and we presented a first test of the co-triad quantization by studying a quantization of the inverse scale factor which can be expressed in terms of the co-triad. As we have seen, applying Thiemann's identity leads to a bounded operator while preserving the correct classical limit. Although quantization ambiguities like factor ordering problems do not affect the classical limit, the outcome of the correct classical limit is not trivial. A look at the eigenvalues (13) reveals that a large-j behavior $V_j \sim j^{d/2}$ leads to $m_{II,j} \sim j^{-d/6} \sim V_j^{-1/3}$, which is needed for the correct classical limit of the inverse scale factor, only for $d=3$. Also the prefactor is important because otherwise the product $V_j^{1/3} m_{II,j}$ would not approach 1 for large j. For this it was necessary to use the correct symplectic structure (1) and also to correct the volume spectrum (4). The quantization techniques of [12] are working perfectly in our quantization which should also increase our confidence in the quantization of the Hamiltonian constraint in the full theory.

An expansion for large j showed the correct classical behavior (14); but the situation is even better than expected: such an expansion is supposed to break down for j being of the order 1, but Fig. 2 shows that the eigenvalues of the inverse scale factor are close to the classical expectation even down to $j=1$. In fact, there is a cancellation in the j^{-1}-correction to the classical expression in Eq. (14), but this still cannot explain the good behavior for $j=1$: the Taylor expansion of Eq. (13) around $x=0$ for $x:=j^{-1}$, which has been used in Eq. (14), does not converge for $x=1$ corresponding to the $j=1$-eigenvalue. This fact shows that a non-perturbative treatment is mandatory: a perturbative expansion in j^{-1}, which is meaningful for large scale factors, breaks down at the Planck scale.

Close to the classical singularity, quantization ambiguities do affect the eigenvalues quantitatively, but not the qualitative conclusion of a nondiverging behavior of the inverse scale factor. One can draw lessons from our quantization, e.g., one could replace the objects $-h[h^{-1}, \hat{V}]$ by $[h, \hat{V}]$ in isotropic models because all edges are closed there and both correspond to the same classical Poisson bracket (this has been done in [9] for simplicity). In the full theory, this is not possible because any edge appearing in a holonomy has to be traced back. One can see that such a replacement would not lead to the desired properties for the inverse scale factor in isotropic models because the resulting expression would not commute with the volume operator (which it should because both only depend on metrical variables). Thus, one has to use the same procedure as in the full theory despite a larger initial freedom.

A consequence of the particular quantization presented in

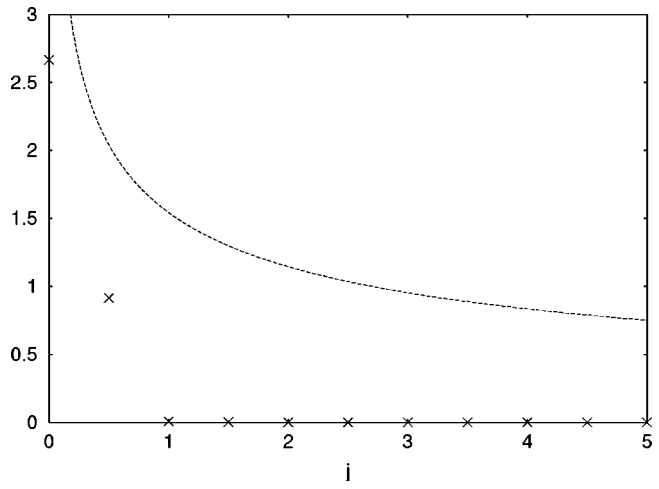

FIG. 4. Eigenvalues of the off-diagonal components of $\hat{m}_{IJ}$ compared to the classical inverse scale factor (dashed line).

Sec. III is the fact that the metric eigenvalues form a non-diagonal matrix even for an isotropic model. The off-diagonal terms are, however, only of the order $l_{\rm p}^4/a^4$ and so do not affect the classical limit (see Fig. 4). Their precise value depends on the factor ordering and other ambiguities which cannot be fixed by studying the classical limit. For example, they can be removed by quantizing the product of the co-triads by

$$\begin{aligned}&\mathrm{tr}(\tau_i h_I[h_I^{-1},\sqrt{\hat{V}}]\,\mathrm{tr}(\tau_i h_J[h_J^{-1},\sqrt{\hat{V}}])\\&\quad=\tfrac{1}{2}\mathrm{tr}(h_I[h_I^{-1},\sqrt{\hat{V}}](h_J[h_J^{-1},\sqrt{\hat{V}}])^{-1})\\&\qquad-\tfrac{1}{4}\mathrm{tr}(h_I[h_I^{-1},\sqrt{\hat{V}}])\,\mathrm{tr}(h_J[h_J^{-1},\sqrt{\hat{V}}])\end{aligned}\quad(21)$$

instead of Eq. (11). Here we used the identity $(\tau_i)^A{}_B(\tau_i)^C{}_D=\frac{1}{2}\epsilon^{AC}\epsilon_{BD}-\frac{1}{4}\delta^A{}_B\delta^C{}_D$ and defined $(h^{-1})^A{}_B:=\epsilon^{AC}\epsilon_{BD}h^D{}_C$. The latter is an identity for the inverse of h if $h\in SU(2)$, but the commutator $h_J[h_J^{-1},\sqrt{\hat{V}}]$ is in general not invertible as an (operator valued) 2×2-matrix. Therefore, $(h_J[h_J^{-1},\sqrt{\hat{V}}])^{-1}$ is just a short form for

$$\begin{aligned}((h_J[h_J^{-1},\sqrt{\hat{V}}])^{-1})^A{}_B&:=\epsilon^{AC}\epsilon_{BD}(h_J[h_J^{-1},\sqrt{\hat{V}}])^D{}_C\\&=(h_J^{-1})^F{}_B[(h_J)^A{}_F,\sqrt{\hat{V}}]\\&=[\sqrt{\hat{V}}-\cos(\tfrac{1}{2}c)\sqrt{\hat{V}}\cos(\tfrac{1}{2}c)\\&\quad-\sin(\tfrac{1}{2}c)\sqrt{\hat{V}}\sin(\tfrac{1}{2}c)]\delta^A{}_B\\&\quad+2\Lambda^A{}_B[\sin(\tfrac{1}{2}c)\sqrt{\hat{V}}\cos(\tfrac{1}{2}c)\\&\quad-\cos(\tfrac{1}{2}c)\sqrt{\hat{V}}\sin(\tfrac{1}{2}c)].\end{aligned}$$

The subtraction of the product of traces in Eq. (21) leads to a cancellation of the off-diagonal components in the resulting $\hat{m}_{IJ}$. However, there is no independent argument in favor of Eq. (11) or Eq. (21) besides the vanishing of off-diagonal components since both expressions have the same classical limit. Off-diagonal components may have relevance in deviations from the Lorentz-invariant vacuum structure because a non-diagonal metric at small scales leads to anisotropies and so to birefringence effects in the propagation of waves. In this context, it may be interesting that the corrections are only of fourth order in the Planck length.

The main result of this paper is that the divergence of the inverse scale factor is completely cured by the quantization methods of quantum geometry, most importantly those developed in [12]. This fact opens up a new way for a resolution of the classical singularity in quantum cosmology [15] which will be investigated in more detail elsewhere [16]. Technically, this comes from an absorption of V^{-1} into a Poisson bracket which is the same procedure which allows matter Hamiltonians to be quantized to densely defined operators [13]. Therefore, *it is the same mechanism which regularizes ultraviolet divergencies in quantum field theories and removes the classical singularity in quantum cosmology*. In particular, geometry itself is responsible for this, and not matter effects.

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