Homogeneous Loop Quantum Cosmology

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Abstract

Loop quantum cosmological methods are extended to homogeneous models in diagonalized form. It is shown that the diagonalization leads to a simplification of the volume operator such that its spectrum can be determined explicitly. This allows the calculation of composite operators, most importantly the Hamiltonian constraint. As an application the dynamics of the Bianchi I model is studied and it is shown that its loop quantization is free of singularities.

1 Introduction

In applications so far, quantum gravity has mostly been analyzed in mini- or midi-superspace models which are obtained by ignoring an infinite number of degrees of freedom of the full theory. In particular, as a first approximation of our universe, which is homogeneous and isotropic at large scales, one often uses a model with a single gravitational degree of freedom, the scale factor or radius \( a \) of an isotropic universe \([1]\). To study more realistic models, and to see whether results of the highly symmetric approximation are robust, one has to break some of the symmetries. As a first step, one can break isotropy while retaining homogeneity. This provides a large class of models much more general than the isotropic ones which still have a finite number of degrees of freedom such that field theoretic complications can be avoided.

The main question for quantum cosmology is the fate of the classical singularity. In isotropic loop quantum cosmology \([2]\) the evolution has been shown to be singularity-free \([3]\), and to lead to additional unexpected quantum effects \([4, 5]\). To check the robustness of those results one has to see whether they persist in less symmetric, e.g. homogeneous, models. At the same time, homogeneous models show many different effects in their classical approach to the singularity which may obtain quantum modifications. Homogeneous models also provide a hint at the behavior of the full theory: according to the BKL-scenario \([6]\) different points on a space-like slice decouple from each other when one approaches the

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singularity which suggests that it is enough to understand homogeneous models in order to see the fate of the classical singularity. Of course, the BKL-scenario itself is not established and so far it is purely classical. Still, the behavior of homogeneous models can provide suggestions as to the general approach to a classical singularity before we are able to study this issue in the full theory.

Besides the reduction of degrees of freedom, the main simplification of isotropic loop quantum cosmology as compared to full quantum geometry is the fact that its volume operator is simple and its spectrum is known explicitly [7]. This is essential for direct computations since the volume operator plays an important role in constructing more complicated operators such as the Hamiltonian constraint [8]. If one can deal with the volume operator easily, one can also obtain an explicit Hamiltonian constraint equation which then can at least be implemented numerically. This has been essential in recent physical applications of isotropic loop quantum cosmology [9, 3, 10, 5, 11, 12]. Homogeneous models [13] still have a finite number of degrees of freedom, but their volume operator corresponds to that of the full theory restricted to a spin network vertex with six incoming edges [7]. It is impossible to compute the spectrum of this operator explicitly since it would require a diagonalization of arbitrarily large matrices.

However, this volume operator is that of a general homogeneous model which has six kinematical gravitational degrees of freedom (all components of a symmetric $3 \times 3$-matrix which represents the metric in a given point). In classical and standard quantum cosmological analyses one usually considers only diagonalized models with only the three diagonal components as kinematical degrees of freedom. Because the remaining components can be chosen to be zero by fixing gauge or symmetry transformations (depending on the model [14]), diagonalized models are enough for physical applications. Diagonalizing a homogeneous model is a restriction to a submodel since some degrees of freedom are ignored. In its physical interpretation this is different from a symmetry reduction, but the same techniques (developed in [15]) apply.

It turns out that this reduction suffices to simplify the volume operator resulting in an explicitly known spectrum. As in the isotropic case, this also requires to deal with generalized spin network states which do not appear as functions on a group manifold. One can represent those states in a convenient form such that an explicit analysis of homogeneous models is possible. The main application in the present paper is the result that the evolution of homogeneous models is non-singular, which occurs in a way very similar to that in isotropic models. This is illustrated here in the Bianchi I model corresponding to a torus action of the symmetry group.

Compared to isotropic models, the absence of a singularity in homogeneous models relies quite non-trivially on properties of quantum geometry. In isotropic models it has been seen to be important that quantum geometry is based on triad variables rather than the metric. This introduces a sign in the degree of freedom corresponding to the metric which is necessary to follow the evolution through the singularity. In homogeneous models we will observe the same effect, but it could also have been obtained if quantum geometry would be based on, e.g., the co-triad rather than the densitized triad. We will see that the removal of homogeneous singularities (contrary to isotropic singularities) would not happen
generically in a theory based on the co-triad. The reason is that the classical singularity lies in the interior of a minisuperspace built from the densitized triad, while it lies at the boundary (at infinity) of a minisuperspace based on the co-triad.

After demonstrating how the diagonalization of a homogeneous model can be done in a connection formulation we will implement it at the quantum level. This requires a reduction of general homogeneous models along the lines of a symmetry reduction which is carried out explicitly. In this way we will obtain the kinematical framework whose structure is very similar to that of isotropic models, and derive the volume operator and its spectrum. This will allow us to compute the Hamiltonian constraint equation explicitly and to bring it into the form of a partial difference equation after transforming to the triad representation. As an application the classical singularity is shown to be absent.

2 Diagonal Bianchi Class A Models

Bianchi models are obtained by a symmetry reduction of general relativity with respect to a symmetry group $S$ which acts freely and transitively on the space manifold $\Sigma \cong S$. Only class A models which have a symmetry group with structure constants fulfilling $c^I_{IJ} = 0$ are amenable to a Hamiltonian analysis. The action provides left-invariant 1-forms $\omega^I_a$ which yield the decomposition $A^i_a = \phi^i_j \omega^I_a$ of an invariant connection with constant coefficients $\phi^i_j$. While the left-invariant 1-forms are regarded as background structure (provided by the symmetry group) with respect to which the reduction is being done, the components $\phi^i_j$ describe the invariant connection in a reduced model. A corresponding decomposition of the densitized triad is given by $E^a_i = p^I_i X^a_i$ where $X^a_i$ are densitized left-invariant vector fields dual to the 1-forms. The symplectic structure of the reduced model is given by $\{\phi^i_j, p^J_k\} = \gamma \delta^i_j \delta^k_l$ where $\gamma$ is the Barbero–Immirzi parameter and $\kappa = 8\pi G$ the gravitational constant. (The role of a possible coordinate volume is discussed in [16].)

In this form, the invariant connection has nine independent components which, after subtracting three gauge degrees of freedom, yields six gauge-invariant components. This corresponds to the fact that a homogeneous model is described by $\phi^i_j$ in full generality without restricting to diagonal metrics. To perform the diagonalization we rewrite an invariant connection by using the polar decomposition $\phi = R\psi$ where $R \in SO(3)$ is a rotation matrix and $\psi$ a symmetric matrix. The symmetric matrix $\psi = \Lambda \text{diag}(c_1, c_2, c_3) \Lambda^T$ can then be diagonalized introducing another rotation matrix $\Lambda \in SO(3)$. Defining $O := RA \in SO(3)$ and redefining $\omega^I_a := \omega^I_a O^K$ we obtain

$$A^i_a = \phi^i_j \omega^I_a = R^i_j \psi^i_j \omega^I_a = R^i_j \Lambda^K J c(K) \Lambda^K J \omega^I_a = c(K) \Lambda^K J \omega^I_a.$$  

Now we can clearly see that only three gauge-invariant degrees of freedom $c_I$ remain, which is just what we need for the diagonalization. (Note that we absorbed the rotation matrix $O$ into the left-invariant 1-forms, which can be done in general without amounting to a reduction of the theory. In a reduced model, however, we have to fix the 1-forms in the beginning as a background structure, and then different forms differing by a rotation.
would lead to different formulations of a model. This explains that the diagonalization leads to a reduction of the model, while any connection can be written in the form \[ D_I = c_{IK}^I \phi^J p^K_I = c_{IK}^J c_{JL}^K p^L_I \delta^K_I \] vanishes identically in the diagonalized class A models whereas it generates inner automorphisms of the symmetry group in non-diagonal models.

In fact, the corresponding decomposition

\[ E^a_i = p^{(K)} \Lambda^I_i X^a_K \]  

of the triad shows that the metric is diagonal. We have to allow negative values for the coefficients \( p^I \) since the triad can have two different orientations while the orientation of \( \Lambda \in SO(3) \) is fixed. The \( SO(3) \)-matrix \( \Lambda \) contains purely gauge degrees of freedom and plays the same role as the matrix \( \Lambda \) in the isotropic decomposition \[2\], even though it arose in a different way. The advantage of the diagonalization in the connection formulation is that gauge-invariant degrees of freedom in \( c_I \) and gauge degrees of freedom in \( \Lambda \) are strictly separate (except for simple residual gauge transformations acting on the \( c_I \), and correspondingly on \( p^I \), which will be discussed in Sec. 3.1). As in the isotropic case, this will lead to a simplification of the volume operator since essentially \( SU(2) \)-calculations can be reduced to \( U(1) \)-calculations. In the diagonal components the symplectic structure is

\[ \{ c_I, p^I \} = \gamma \kappa \delta^I_I. \]  

Also the co-triad \( e^i_a = a^i_J \omega^J_a = a^i_J \Lambda^J_i \omega^J_a \) has the diagonal form with arbitrary real parameters \( a_I \in \mathbb{R} \). The relation between the triad and co-triad components follows from \( E^a_i = |\det e| (e^i_a)^{-1} \) and is given by

\[ p^1 = |a_2a_3| \text{sgn}(a_1), \quad p^2 = |a_1a_3| \text{sgn}(a_2), \quad p^3 = |a_1a_2| \text{sgn}(a_3). \]  

In these variables the volume is given by

\[ V = \sqrt{|\frac{1}{6} e^{ijk} e_{JIK} p^J_i p^K_j|} = \sqrt{|p^1 p^2 p^3|} = |a_1a_2a_3|. \]

For the geometrical interpretation of the connection components we need the homogeneous spin connection \( \Gamma^i_a = \Gamma^i_{(I)} \Lambda^I_i \omega^J_a \). From the general formula \[17\]

\[ \Gamma^i_a = -\frac{1}{2} e^{ijk} e_{JIK} (2 \partial_J a^k e_b^k + e_c^k e_d^l \partial_a e^l \partial_b e^d) \]

we derive

\[ \Gamma^i = \frac{1}{2} \left( \frac{a_I}{a_K} n^J + \frac{a_K}{a_I} n^K - \frac{a_I^2}{a_J a_K} n^I \right) \]

\[ = \frac{1}{2} \left( \frac{p^K_J}{p^I_K} n^J + \frac{p^I_K}{p^K_J} n^K - \frac{p^J I}{(p^I)^2} n^J \right) \quad \text{for } \epsilon_{IJK} = 1 \]
where the numbers \( n^I \) specify the Bianchi model via \( c^I_{JK}\kappa = \epsilon_{JKL}n^L = \epsilon^I_{JK}n^{(I)} \). Only the Bianchi I model has vanishing spin connection; otherwise \( \Gamma_i \) depends on the triad components, contrary to isotropic models where spin connection components are constant.

For diagonal models the Euclidean part of the Hamiltonian constraint \([18, 19]\) reduces to

\[
H^{(E)} = -\kappa^{-1} \det(e^i_j)^{-1}(\epsilon_{ijk}F^i_{t,j}E^j_i E^j_k)
\]

\[
= \kappa^{-1} \det(a^i_j)^{-1}(\epsilon_{ijk}e^K_i K^j_k p^j_k - \phi^i_j \phi^i_k p^j_k + \phi^i_j \phi^i_k p^j_k)
\]

\[
= 2\kappa^{-1} \left((n^1 c_1 - c_2 c_3) a_1 + (n^2 c_2 - c_1 c_3) a_2 + (n^3 c_3 - c_1 c_2) a_3\right).
\]

The full constraint \( H = -H^{(E)} + P \) with

\[
P = -2(1 + \gamma^2)\kappa^{-1} \det(e^i_j)^{-1} K^i_j K^j_i E^i_j E^j_i,
\]

using the extrinsic curvature \( K^i_j = \gamma^{-1}(\Gamma^i_j - \phi^i_j) \), is

\[
H = 2\kappa^{-1} \left(((c_2 \Gamma_3 + c_3 \Gamma_2 - \Gamma_3 \Gamma_2)(1 + \gamma^2) - n^1 c_1 - \gamma^2 c_2 c_3) a_1
+ ((c_1 \Gamma_3 + c_3 \Gamma_1 - \Gamma_1 \Gamma_3)(1 + \gamma^2) - n^2 c_2 - \gamma^2 c_1 c_3) a_2
+ ((c_1 \Gamma_2 + c_2 \Gamma_1 - \Gamma_1 \Gamma_2)(1 + \gamma^2) - n^3 c_3 - \gamma^2 c_1 c_2) a_3\right).
\]

In terms of extrinsic curvature components \( K^i_j = \frac{1}{2} \dot{a}_l = \gamma^{-1}(\Gamma^i_l - \phi^i_l) \), where the dot indicates a derivative with respect to proper time \( t \) corresponding to lapse \( N = 1 \), it reads

\[
H = 2\kappa^{-1} \left(((\Gamma_2 \Gamma_3 - n^1 \Gamma_1) a_1 + (\Gamma_1 \Gamma_3 - n^2 \Gamma_2) a_2 + (\Gamma_1 \Gamma_2 - n^3 \Gamma_3) a_3
- \frac{1}{4} (a_1 \dot{a}_2 \dot{a}_3 + a_2 \dot{a}_1 \dot{a}_3 + a_3 \dot{a}_1 \dot{a}_2)\right)
\]

which yields the Hamiltonian constraint equation \( H + H_{\text{matter}}(a_1, a_2, a_3) = 0 \) as a differential equation for the co-triad components \( a_1 \).

As special cases we obtain isotropic models if we set \( a_1 = a_2 = a_3 = \alpha \) such that

\[
H + H_{\text{matter}}(a) = -\frac{3}{2} \kappa^{-1}(\dot{a}^2 + 2\Gamma)a + H_{\text{matter}}(a) = 0
\]

where \( \Gamma = 0 \) for the flat model and \( \Gamma = \frac{1}{2} \) for the model with positive spatial curvature. In this case, the Hamiltonian constraint equation is the Friedmann equation.

An example for an anisotropic model is the vacuum Bianchi I model where \( n^I = 0 \) and \( H_{\text{matter}} = 0 \). Therefore, the constraint equation reads

\[
a_1 \dot{a}_2 \dot{a}_3 + a_2 \dot{a}_1 \dot{a}_3 + a_3 \dot{a}_1 \dot{a}_2 = 0.
\]

A simple solution is the one where the \( a_I \) are constant such that all terms in the constraint equation vanish separately; this solution is Minkowski space. All other solutions are given by the well-known Kasner solutions \([20]\) \( a_I \propto t^{\alpha_I} \) where the constant exponents \( \alpha_I \) have to satisfy \( \sum I \alpha_I = 1 = \sum I \alpha^2_I \). These relations can be fulfilled only for \(-1 < \alpha_I \leq 1\) and, furthermore, one coefficient \( \alpha_I \) has to be negative while the other two are positive.
This leads to an evolution of the form of Kasner epochs where one direction of space is contracting while the other two are expanding. The total volume \( V = a_1a_2a_3 \propto t \) always increases monotonically. In these co-triad (or metric) variables \( a_I \) the structure of the singularity at \( t = 0 \) is quite complicated because one metric component diverges. This implies that the classical singularity lies at the boundary of minisuperspace.

In the densitized triad variables \( p^I \) on which the loop quantum cosmological description is based the situation turns out to be different. Using the relation between co-triad and densitized triad components and the relations for the coefficients \( \alpha_I \) it follows that \( p^I \propto t^{1-\alpha_I} \) which has always a positive exponent. Thus, the triad components are always increasing and the singularity lies at \( p^I = 0 \) which is an interior point of minisuperspace. This will turn out to be crucial for the generic removal of the classical singularity.

Other Bianchi models have a non-vanishing potential given by the spin connection components. This leads to possible changes in the expansion/contraction behavior of the co-triad components with intermediate regimes approximately described by Kasner epochs. Such a succession of different epochs can even be chaotic in certain models which renders the structure of the classical singularity even more complicated. In densitized triad variables, the situation looks again simpler since all components decrease during any Kasner epoch approaching the singularity. Only the component which decreases the fastest changes during the succession of different epochs.

3 Quantum Theory of Diagonal Bianchi Class A Models

According to the general scheme of a symmetry reduction for diffeomorphism invariant quantum field theories of connections [15], symmetric states are distributional states which are supported only on invariant connections with respect to the given symmetry group. For homogeneous models those states are in one-to-one correspondence with functions on the group manifold \( SU(2)^3 \) which can be visualized as spin network states associated with a graph containing a single vertex and three closed edges intersecting in the 6-vertex. For the diagonalization we have to perform an additional reduction to diagonal homogeneous connections [14]. Even though this is not a symmetry reduction, the same techniques apply. Consequently, diagonal homogeneous states are functions on the manifold

\[
\{(\exp(c_1\Lambda_1^i\tau_i), \exp(c_2\Lambda_2^i\tau_i), \exp(c_3\Lambda_3^i\tau_i)) : c_I \in \mathbb{R}, \Lambda \in SO(3)\} \subset SU(2)^3
\]  

which is obtained by building (point) holonomies out of the connection components (this issue is discussed more carefully in [16]). The diagonal homogeneous configuration space is by definition a submanifold of the general homogeneous configuration space \( SU(2)^3 \), but as in the isotropic case [7] one can easily check that it is not a subgroup. This implies that the Peter–Weyl theorem cannot be used to find a generating set of functions, and states have to be expected not to be ordinary spin network states. In the isotropic case all possible functions of the lone gauge invariant connection component \( c \) were allowed as
gauge invariant states, not just even functions as would be expected by a naive reduction (corresponding to characters on a single copy of $SU(2)$).

3.1 Diagonal Homogeneous Spin Network States and Basic Operators

To derive all possible states for a given model one has to restrict the already known homogeneous states (or in general all states of the full theory) to the subspace of reduced connections, find an independent set, and complete it with respect to the measure on the space of reduced connections. The resulting set can be orthonormalized to derive a generalized spin network basis. In most cases this procedure can be simplified if a decomposition of reduced connections into pure gauge degrees of freedom and remaining components is known. Then, gauge invariant states can be found to be arbitrary functions of the remaining components subject possibly to residual gauge transformations which are usually discrete and easy to find. For instance, in the isotropic case an invariant connection has the form $A_i^g = c \Lambda_i^g \omega_i^g$ where the components $\Lambda_i^g$ are pure gauge. There are no residual gauge transformations on $c$ (note that changing the sign of $c$ is equivalent to changing the orientation of $\Lambda$, which is not a gauge transformation) such that gauge invariant states can be arbitrary functions of $c$ without restrictions. This basic fact turns out to have important consequences even for the dynamics and physical applications: it implies that states are labeled by an integer quantum number $n$ rather than a positive integer $2j + 1$ as would be expected for an $SU(2)$-theory. In the end, this leads to the removal of classical singularities in isotropic models.

We can now perform this analysis for diagonal homogeneous connections (1) which also allow a decomposition into pure gauge degrees of freedom $\Lambda_i^g$ and remaining components $c_I$. We start with noting the measure on the space of gauge invariant diagonal homogeneous connections as a quotient of (9). Since the relations between the three copies of $SU(2)$ implied by the diagonalization only affect the gauge degrees of freedom $\Lambda_i^g$, the gauge invariant measure is a direct product of three copies of the Haar measure on $SU(2)$. Therefore, we use

$$d\mu(c_1, c_2, c_3) = (2\pi)^{-3} \sin^2(\frac{1}{2}c_1) \sin^2(\frac{1}{2}c_2) \sin^2(\frac{1}{2}c_3) dc_1 dc_2 dc_3.$$  (10)

Gauge invariant states have to be functions of $c_I$, but this time there are residual gauge transformations: it can be seen from (5) that one can change the sign of two components $c_I$ simultaneously while keeping the third one fixed (e.g., a gauge transformation with $\exp(\pi \Lambda_i^g \tau_i)$ changes the sign of $c_1$ and $c_2$). Those are the only residual gauge transformations such that gauge invariant states have to be invariant under changing two signs of the $c_I$.

To write down a basis we use the isotropic states given by

$$\chi_j(c) = \frac{\sin(j + \frac{1}{2})c}{\sin \frac{1}{2}c}, \quad j \in \frac{1}{2}\mathbb{N}_0$$  (11)
together with \( \zeta_{-\frac{1}{2}}(c) = (\sqrt{2} \sin \frac{1}{2} c)^{-1} \) and

\[
\zeta_j(c) = \frac{\cos(j + \frac{1}{2})c}{\sin \frac{1}{2} c}, \quad j \in \frac{1}{2} \mathbb{N}_0
\] (12)

which are orthonormalized with respect to the measure \( d\mu(c) = (2\pi)^{-1} \sin^2(\frac{1}{2} c) dc \). Thus, all orthonormal states of the diagonal homogeneous model can be written as

\[
\chi_{j_1,j_2,j_3}(c_1, c_2, c_3) := \chi_{j_1}(c_1) \chi_{j_2}(c_2) \chi_{j_3}(c_3), \quad \zeta_{j_1,j_2,j_3}(c_1, c_2, c_3) := \zeta_{j_1}(c_1) \zeta_{j_2}(c_2) \zeta_{j_3}(c_3)
\] (13)

where the \( j_I \) can be \(-\frac{1}{2}\) only for \( \zeta \). As in the isotropic case, we obtain twice as many states as expected from positive spin labels. Such a doubling of the number of states has been seen to be necessary in the isotropic model because it yields eigenvalues for the triad operator corresponding to the two different triad orientations. To verify this in the diagonal homogeneous model we have to consider the quantization of the triad components \( p^I \).

As in [7], invariant vector field operators which quantize triad components in the full homogeneous model reduce to the self-adjoint derivative operators

\[
\hat{p}^I = -i\gamma^2_p \left( \frac{\partial}{\partial c^I} + \frac{1}{2} \cot(\frac{1}{2} c^I) \right).
\] (14)

These operators, however, do not leave the space of states (13) invariant corresponding to the fact that the triad components \( p^I \) are not gauge invariant. As with connection components, we can change two signs of the \( p^I \) simultaneously by a gauge transformation. Thus, only \( |p^I| \) and \( \text{sgn}(p^1 p^2 p^3) \) are gauge invariant, the latter quantity being the orientation. Still, for calculations it is convenient to work with the non-gauge invariant \( p^I \)-operators and to use their eigenstates which have to be non-gauge invariant. These eigenstates can easily be seen to be

\[
|n_1, n_2, n_3 \rangle := |n_1 \rangle \otimes |n_2 \rangle \otimes |n_3 \rangle
\] (15)

where

\[
\langle c | n \rangle = \frac{\exp(\frac{1}{2} inc)}{\sqrt{2} \sin(\frac{1}{2} c)}
\]

are the isotropic \( p \)-eigenstates in the connection representation. Using Euler’s formula for the exponential shows that the eigenstates (15) are not linear combinations of the gauge invariant states (13) only. A gauge invariant state can be expanded in the states (15) as

\[
|s \rangle = \sum_{n_1, n_2, n_3} s_{n_1, n_2, n_3} |n_1, n_2, n_3 \rangle
\] (16)

where the coefficients \( s_{n_1, n_2, n_3} \), which represent the state in the triad representation, have to fulfill

\[
s_{n_1, n_2, n_3} = s_{-n_1, -n_2, n_3} = s_{n_1, -n_2, -n_3} = s_{-n_1, n_2, -n_3}.
\] (17)
The set of basic operators is completed by quantizing the connection components which has to be done via (point) holonomies $h_I = \exp(c_I \Lambda^I_\tau) = \cos(\frac{1}{2}c_I) + 2\Lambda^I_\tau \sin(\frac{1}{2}c_I)$ as multiplication operators. The matrix $\Lambda$ is not gauge invariant, as a multiplication operator, and does not even leave the space of states (15) invariant. Nevertheless, we do not need to extend our state space once more because, as shown in (9), $\Lambda$ drops out of gauge invariant operators even when holonomies are used in intermediate steps (as in commutators with the volume operator). We then need only the action of $\cos(\frac{1}{2}c_I)$ and $\sin(\frac{1}{2}c_I)$ which can readily be seen to be

\[
\begin{align*}
\cos(\frac{1}{2}c_I)|n_1, n_2, n_3\rangle &= \frac{1}{2}(|n_1 + 1, n_2, n_3\rangle + |n_1 - 1, n_2, n_3\rangle) \\
\sin(\frac{1}{2}c_I)|n_1, n_2, n_3\rangle &= -i\frac{1}{2}(|n_1 + 1, n_2, n_3\rangle - |n_1 - 1, n_2, n_3\rangle)
\end{align*}
\]

and correspondingly for $c_2$ and $c_3$.

### 3.2 Gauge Invariant Triad Operators

As already discussed, the triad components $p^I$ are not completely gauge invariant, but only the functions $|p^I|$ and $\text{sgn}(p^1 p^2 p^3)$ are. The corresponding operators must leave the gauge invariant states (15) invariant. In fact, we have

\[
\begin{align*}
\hat{p}^I|\chi_{j_1,j_2,j_3}\rangle &= \gamma l_P^2 (j_I + \frac{1}{2}) \chi_{j_1,j_2,j_3} \quad \text{and} \\
\hat{p}^I|\zeta_{j_1,j_2,j_3}\rangle &= \gamma l_P^2 (j_I + \frac{1}{2}) \zeta_{j_1,j_2,j_3}
\end{align*}
\]

and

\[
\begin{align*}
\hat{p}^1 \hat{p}^2 \hat{p}^3 \chi_{j_1,j_2,j_3} &= i(\gamma l_P^2)^3 (j_1 + \frac{1}{2})(j_2 + \frac{1}{2})(j_3 + \frac{1}{2}) \chi_{j_1,j_2,j_3} \\
\hat{p}^1 \hat{p}^2 \hat{p}^3 \zeta_{j_1,j_2,j_3} &= -i(\gamma l_P^2)^3 (j_1 + \frac{1}{2})(j_2 + \frac{1}{2})(j_3 + \frac{1}{2}) \zeta_{j_1,j_2,j_3}.
\end{align*}
\]

Simultaneous eigenstates of all gauge invariant triad operators are given by

\[
2^{-\frac{1}{2}}(\zeta_{j_1,j_2,j_3} \pm i\chi_{j_1,j_2,j_3}).
\]

In terms of the states (15) the action reads

\[
|\hat{p}^I| |n_1, n_2, n_3\rangle = \frac{1}{2}\gamma l_P^2 |n_I| |n_1, n_2, n_3\rangle
\]

and

\[
\text{sgn}(\hat{p}^1 \hat{p}^2 \hat{p}^3)|n_1, n_2, n_3\rangle = \text{sgn}(n_1 n_2 n_3) |n_1, n_2, n_3\rangle.
\]

Gauge invariant simultaneous eigenstates are

\[
\begin{align*}
\frac{1}{2}(|n_1, n_2, n_3\rangle &+ | - n_1, - n_2, n_3\rangle + | - n_1, n_2, - n_3\rangle + |n_1, - n_2, - n_3\rangle) \\
&= 2^{-\frac{1}{2}} \left( \frac{1}{2} |n_1-1, n_2-1, n_3\rangle + i \text{sgn}(n_1 n_2 n_3) \chi_{\frac{1}{2} |n_1-1, n_2-1, n_3|} \right)
\end{align*}
\]

From the triad operators we can immediately build the volume operator $\hat{V} = \sqrt{|\hat{p}^I \hat{p}^2 \hat{p}^3|}$ (it can also be derived from the non-diagonal homogeneous volume operator (7), which itself descends from the full one) with eigenvalues

\[
\hat{V}|n_1, n_2, n_3\rangle = (\frac{1}{2}\gamma l_P^2)^\frac{3}{2} \sqrt{|n_1 n_2 n_3|} |n_1, n_2, n_3\rangle =: V_{n_1, n_2, n_3} |n_1, n_2, n_3\rangle.
\]
To avoid confusion we note that the isotropic states $|n\rangle$ of [2] are not to be identified with states $|n, n, n\rangle$. Rather, according to the general scheme of a symmetry reduction an isotropic state would correspond to a distributional state in a homogeneous model and thus be non-normalizable. Therefore, the isotropic volume eigenvalues need not be given by $V_{n,n,n}$.

Using the basic operators we can construct more complicated ones like inverse metric operators along the lines of [8, 21, 9]. Since there are no essential differences to the calculations in the isotropic model, we will not repeat details here. Those operators are needed when one quantizes the spin connection (5) or matter Hamiltonians.

4 Dynamics of the Bianchi I Model

So far we considered only kinematical aspects, which are independent of the particular type of Bianchi model. Specific properties only enter via the Hamiltonian constraint (7) (or the spin connection) which explicitly contains the structure constants of the symmetry group. Bianchi models usually have a non-vanishing spin connection which is necessary to yield non-zero intrinsic curvature. In the full theory such a statement would be meaningless because the spin connection does not have an invariant meaning. More precisely, it can be made arbitrarily small locally by choosing appropriate coordinates. In symmetric models, however, we are restricted to coordinate choices which respect the symmetry such that the spin connection does have a coordinate independent meaning in homogeneous models (or certain components in a less symmetric model). This also implies that it is impossible to ignore the effects of a possibly large spin connection whenever there is non-zero intrinsic curvature. As a consequence, even in classical regimes where, e.g., the extrinsic curvature is small, there can still be large intrinsic curvature contributions. Since this effect is a consequence of the symmetry and is not present in the full theory, it has to be dealt with appropriately. For instance, it affects the quantization of the Hamiltonian constraint (which has not been taken properly into account for the general quantization of the Hamiltonian constraints in homogeneous models presented in [22]) and the interpretation of the semiclassical limit; this is discussed in more detail in [23].

The lone exception to the preceding statements is the Bianchi I model which has vanishing intrinsic curvature and where the spin connection is always zero. Consequently, its quantization is simpler and also closer to that of the full theory [8]. In the present paper we restrict our attention to this model and in particular to the issue of the classical singularity displayed in the Kasner behavior.

4.1 Hamiltonian Constraint

From [22] we obtain the quantized Euclidean part of the Hamiltonian constraint in the form

$$\hat{H}^{(E)} = 4i(\kappa l_P^2)^{-1} \sum_{IJK} \epsilon^{IJK} \text{tr}(h_I h_J h_K^{-1} h_I^{-1} h_J^{-1} h_K^{-1} [\hat{h}_K^{-1}, \hat{V}]) .$$
A further simplification of the Bianchi I model is that the Lorentzian constraint is related to the Euclidean part simply by \( H = \gamma^{-2}H^{(E)} \) which we make use of here. Alternatively, one could derive the Lorentzian constraint as in the full theory \(^{[3]}\) by expressing the extrinsic curvature as a commutator of the Euclidean part and the volume. Since this has been done in detail in the isotropic model without yielding essential differences to the simpler approach adopted here \(^{[2]}\), we will not perform the full analysis. In other Bianchi models the relation between the Lorentzian constraint and the Euclidean part is more complicated and one would have to quantize the additional terms (containing the spin connection) by hand, introducing more ambiguities \(^{[23]}\).

Using diagonal (point) holonomies \( h_l = \cos(\frac{1}{2}c_I) + 2\Lambda_l^i \tau_i \sin(\frac{1}{2}c_I) \) in \( \dot{H} := \gamma^{-2}\dot{H}^{(E)} \), we obtain

\[
\dot{H} = 32i\gamma^{-3}\kappa^{-1}l_p^{-2} \left( \sin(\frac{1}{2}c_1) \cos(\frac{1}{2}c_1) \sin(\frac{1}{2}c_2) \cos(\frac{1}{2}c_2) \right. \\
\times \left( \sin(\frac{1}{2}c_3) \dot{V} \cos(\frac{1}{2}c_3) - \cos(\frac{1}{2}c_3) \dot{V} \sin(\frac{1}{2}c_3) \right) \\
+ \sin(\frac{1}{2}c_3) \cos(\frac{1}{2}c_3) \sin(\frac{1}{2}c_1) \cos(\frac{1}{2}c_1) (\sin(\frac{1}{2}c_2) \dot{V} \cos(\frac{1}{2}c_2) - \cos(\frac{1}{2}c_2) \dot{V} \sin(\frac{1}{2}c_2)) \\
\left. + \sin(\frac{1}{2}c_2) \cos(\frac{1}{2}c_2) \sin(\frac{1}{2}c_3) \cos(\frac{1}{2}c_3) (\sin(\frac{1}{2}c_1) \dot{V} \cos(\frac{1}{2}c_1) - \cos(\frac{1}{2}c_1) \dot{V} \sin(\frac{1}{2}c_1)) \right)
\]

with action

\[
\dot{H}|_{n_1, n_2, n_3} = \gamma^{-3}3^{-1}l_p^{-2} ((V_{n_1,n_2,n_3+1} - V_{n_1,n_2,n_3-1})(|n_1 + 2, n_2 + 2, n_3\rangle \\
- |n_1 - 2, n_2 + 2, n_3\rangle) - |n_1 + 2, n_2 - 2, n_3\rangle + |n_1 - 2, n_2 - 2, n_3\rangle) \\
+ (V_{n_1,n_2+1,n_3} - V_{n_1,n_2-1,n_3})(|n_1 + 2, n_2, n_3 + 2\rangle \\
- |n_1 - 2, n_2, n_3 + 2\rangle - |n_1 + 2, n_2, n_3 - 2\rangle + |n_1 - 2, n_2, n_3 - 2\rangle) \\
+ (V_{n_1+1,n_2,n_3} - V_{n_1-1,n_2,n_3})(|n_1 + 2, n_2 + 2, n_3\rangle \\
- |n_1 + 2, n_2, n_3 - 2\rangle - |n_1 - 2, n_2, n_3 - 2\rangle + |n_1, n_2 - 2, n_3 - 2\rangle)) .
\]

To derive an interpretation of the constraint equation \((\dot{H} + \dot{H}_{\text{matter}})|s = 0\) as an evolution equation, we transform to the triad representation \(^{[16]}\) where we have

\[
(\dot{H}s)_{n_1,n_2,n_3} = \gamma^{-3}\kappa^{-1}l_p^{-2} ((V_{n_1-2,n_2-2,n_3+1} - V_{n_1-2,n_2-2,n_3-1}) s_{n_1-2,n_2-2,n_3} \\
- (V_{n_1+2,n_2-2,n_3+1} - V_{n_1+2,n_2-2,n_3-1}) s_{n_1+2,n_2-2,n_3} \\
- (V_{n_1-2,n_2+2,n_3+1} - V_{n_1-2,n_2+2,n_3-1}) s_{n_1-2,n_2+2,n_3} \\
+ (V_{n_1+2,n_2+2,n_3+1} - V_{n_1+2,n_2+2,n_3-1}) s_{n_1+2,n_2+2,n_3} \\
+ (V_{n_1-2,n_2+1,n_3+2} - V_{n_1-2,n_2-1,n_3+2}) s_{n_1-2,n_2,n_3+2} \\
- (V_{n_1+2,n_2+1,n_3+2} - V_{n_1+2,n_2-1,n_3+2}) s_{n_1+2,n_2,n_3+2} \\
- (V_{n_1-2,n_2+1,n_3+2} - V_{n_1-2,n_2-1,n_3+2}) s_{n_1-2,n_2,n_3+2} \\
+ (V_{n_1+2,n_2+1,n_3+2} - V_{n_1+2,n_2-1,n_3+2}) s_{n_1+2,n_2,n_3+2} \\
+ (V_{n_1+1,n_2-2,n_3+2} - V_{n_1-1,n_2-2,n_3+2}) s_{n_1,n_2-2,n_3+2} \\
- (V_{n_1+1,n_2-2,n_3+2} - V_{n_1-1,n_2-2,n_3+2}) s_{n_1,n_2-2,n_3+2} \\
+ (V_{n_1+1,n_2+2,n_3+2} - V_{n_1-1,n_2+2,n_3+2}) s_{n_1,n_2+2,n_3+2}) .
\]
Using the volume eigenvalues $|s\rangle$, we obtain the evolution equation

$$
|n_3 + 2|s\rangle \left( |n_2 + 1|s\rangle - |n_2 - 1|s\rangle \right) \left( |n_1 + 2|s\rangle s_{n_1+2,n_2,n_3+2} - |n_1 - 2|s\rangle s_{n_1-2,n_2,n_3+2} \right) \\
+ \left( |n_1 + 1|s\rangle - |n_1 - 1|s\rangle \right) \left( |n_2 + 2|s\rangle s_{n_1,n_2+2,n_3+2} - |n_2 - 2|s\rangle s_{n_1,n_2-2,n_3+2} \right) \\
+ \left( |n_3 + 1|s\rangle - |n_3 - 1|s\rangle \right) \left( |n_2 - 2|s\rangle |n_1 - 2|s\rangle s_{n_1-2,n_2-2,n_3} - |n_1 + 2|s\rangle s_{n_1+2,n_2-2,n_3} \right) \\
+ |n_2 + 2|s\rangle \left( |n_1 + 2|s\rangle s_{n_1+2,n_2+2,n_3} - |n_1 - 2|s\rangle s_{n_1-2,n_2+2,n_3} \right) \\
+ |n_3 - 2|s\rangle \left( |n_2 + 1|s\rangle - |n_2 - 1|s\rangle \right) \left( |n_1 - 2|s\rangle s_{n_1-2,n_2,n_3-2} - |n_1 + 2|s\rangle s_{n_1+2,n_2,n_3-2} \right) \\
+ \left( |n_1 + 1|s\rangle - |n_1 - 1|s\rangle \right) \left( |n_2 - 2|s\rangle s_{n_1,n_2-2,n_3-2} - |n_2 + 2|s\rangle s_{n_1,n_2+2,n_3-2} \right)
$$

\[= -2\kappa (\frac{\hbar}{cG})^2 H_{\text{matter}}(n_1, n_2, n_3)s_{n_1,n_2,n_3} \tag{23}\]

where $H_{\text{matter}}$ can be any matter Hamiltonian which depends on the triad components $n_I$ and acts on the wave function $s_{n_1,n_2,n_3}$ (we suppressed the dependence of the wave function on matter fields). Equation (23) is a partial difference equation for the wave function in the triad representation. For a dynamical interpretation we have to choose an internal time which in the case of the Bianchi I model can easily be done as one of the diagonal components of the triad, e.g., $n_3$. This is justified because classically $p^3$ is always monotonically expanding or contracting. With this internal time the constraint equation has the form of an evolution equation in a discrete time, as expected on general grounds [24]..

### 4.2 Absence of a Singularity

The classical Kasner behavior suggests that the approach to the singularity of the Bianchi I model can well be described with the internal time $p^3$ (or any other diagonal triad component). In the loop quantization this leads to the discrete internal time $n_3$ which we already chose to interpret Equation (23) as a time evolution equation for the wave function $s_{n_1,n_2,n_3}$. The other labels $n_1$ and $n_2$ can be regarded as independent degrees of freedom evolving in the time $n_3$. While the time variable $n_3$ is unrestricted in the range from $-\infty$ to $+\infty$, for independent values of the wave function we have to consider only non-negative $n_1, n_2 \geq 0$. Remaining values of the wave function are then given by the relations

\[s_{-n_1,n_2,n_3} = s_{n_1,n_2,-n_3} , \quad s_{n_1,-n_2,n_3} = s_{n_1,n_2,-n_3} \]  \[= \tag{24}\]

which follow from gauge invariance. In other words, $s$ can be seen as a function on a discrete space $\{(n_1, n_2, n_3) : n_1, n_2 \in \mathbb{N}_0, n_3 \in \mathbb{Z}\}$ subject to the identifications $(n_1, 0, n_3) \equiv (n_1, 0, -n_3)$ and $(0, n_2, n_3) \equiv (0, n_2, -n_3)$. Certainly, any one of the discrete coordinates can be chosen to take negative values; however, it is most convenient to choose that one which is being used as internal time. As in isotropic loop quantum cosmology, the difference to the classical and Wheeler–DeWitt approach is that there is a “doubling” of minisuperspace.
which comes from the two possible orientations of a triad. This can be obtained in any triad formulation, but the non-trivial fact is whether or not the evolution can be extended meaningfully and uniquely through the boundary corresponding to the classical singularity.

To study this question we use the evolution equation (23). We will interpret this equation as an evolution equation in the internal time $n_3$, but it is important to note that the presence of a singularity is independent of the choice of internal time. The question is whether or not the wave function can be extended uniquely throughout all of minisuperspace even crossing singular hypersurfaces. For an intuitive picture one usually selects a function on minisuperspace, most often the volume, as a time coordinate and views solutions in a semiclassical regime as representing wave packets evolving in this internal time. But this is only necessary for an intuitive interpretation, not for a proof of absence of singularities. In particular, one can choose a time coordinate different from the conventional volume. Here we use the integer $n_3$, corresponding to the triad component $p^3$, because it leads to a difference equation, while the volume does not have equally spaced eigenvalues and thus does not give a simple evolution equation. Physical results, e.g. expectation values of observables, can always be translated between different internal time pictures.

As a recurrence relation, equation (23) does not only require initial conditions at slices of constant $n_3$ but also boundary data for small values of $n_1$ and $n_2$. We will first assume that the correct amount of boundary conditions is given such that we can solve the evolution equation for positive $n_3$ and negative $n_3$, respectively. The issue of initial and boundary conditions will be discussed later.

Starting with initial data at large positive times $n_3$ and evolving backwards, equation (23) can be used as a recurrence relation as long as the coefficient $\sqrt{|n_3 - 2|}$ of the lowest order part, which contains the wave function with label $n_3 - 2$, is non-zero. This is the case only until $n_3 = 2$ such that our initial and boundary data uniquely fix the wave function for all $n_3 > 0$. The values at singular states, identified with $n_3 = 0$ or $n_1 = 0$ or $n_2 = 0$, cannot be determined which looks like a breakdown of the evolution at the classical singularity. However, it turns out, in exactly the same way as in the isotropic case, that we can evolve through the singularity: the values of the wave function at the classical singularity remain undetermined, but since they completely drop out of the evolution equation they are not needed to find the wave function at negative times $n_3$. The initial data chosen at positive $n_3$, together with boundary data, uniquely determine the wave function at positive and negative $n_3$ and the evolution through the classical singularity is perfectly well-defined. Here we also used the fact that matter Hamiltonians quantized with quantum geometrical methods [21] are zero at the classical singularity such that also the right hand side of (23) does not contribute values of the wave function at the classical singularity. Again, it is essential that the orientation of the triad provides us with twice as many states as expected in a metric formulation. Thereby we naturally obtain negative values of our internal time. Still, just using variables which can take negative values is not enough since, most importantly, the evolution must remain well-defined. This is a non-trivial fact which in this case relies in part on the discreteness of the triad minisuperspace. As already alluded to earlier, another non-trivial fact (which is not present in the isotropic case) is
that the classical singularity lies in the interior of minisuperspace in the densitized triad variables which we have to use in quantum geometry, while it would be at the infinite boundary for, e.g., co-triad variables. It would be harder to see in general if a singularity at the boundary of minisuperspace can be eliminated with the present mechanism.

We also note that choosing a different factor ordering of the constraint would lead to a singularity since some values of the wave function could not be determined from the initial data but now would not drop out completely and thus be necessary to determine other values. The ordering we have to use here for a non-singular evolution, corresponding to ordering the triads to the right, is the same as in the isotropic case.

In order to discuss the boundary conditions we first transform the evolution equation by introducing

\[ t_{m_1, m_2, m_3} := V_{2m_1, 2m_2, 2m_3} s_{2m_1, 2m_2, 2m_3} \]

and defining

\[ d(m) := \begin{cases} \sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}} & \text{for } m \neq 0 \\ 0 & \text{for } m = 0 \end{cases} \]  

(25)

Since the volume eigenvalues \( V_{n_1, n_2, n_3} \) vanish for \( n_1 n_2 n_3 = 0 \), the function \( t \) has to fulfill

\[ t_{0, m_2, m_3} = t_{m_1, 0, m_3} = t_{m_1, m_2, 0} = 0 \]

(26)

for all \( m_1, m_2, m_3 \). In addition, \( t \) also has to fulfill the gauge invariance conditions \( \text{(24)} \) such that we can restrict again to non-negative \( m_1, m_2 \). Equation \( \text{(23)} \) then turns into

\[
\begin{align*}
\frac{d(m_2)}{\sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}}} &+ \frac{d(m_1)}{\sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}}} \\
+ \frac{d(m_3)}{\sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}}} &+ \frac{d(m_1)}{\sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}}} \\
&= -\gamma^3 \kappa_P^2 \hat{\rho}_{\text{matter}}(m_1, m_2, m_3) t_{m_1, m_2, m_3}
\end{align*}
\]  

(27)

where

\[ \hat{\rho}_{\text{matter}}(m_1, m_2, m_3) = \hat{H}_{\text{matter}}(m_1, m_2, m_3) / V_{m_1, m_2, m_3} \]

(28)

for non-zero \( m_1, m_2, m_3 \) and zero otherwise, is the matter energy density operator.

Starting with initial data at two slices of constant \( m_3 \) yields via recurrence the combination

\[
\frac{d(m_2)}{\sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}}} + \frac{d(m_1)}{\sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}}}
\]

of values of the wave function at the next step \( m_3 + 1 \). For this to yield unique values \( t_{m_1, m_2, m_3+1} \) we need to specify boundary values at low values of \( m_1 \) and \( m_2 \). For \( m_1 = 0 \) we obtain the values of

\[
\frac{d(m_2)}{\sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}}} = \frac{d(m_2)}{\sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}}}
\]

from which we can find \( t_{1, m_2, m_3} \) at negative \( m_3 \) provided that the values \( t_{1, m_2, m_3} \) for positive \( m_3 \) are given by boundary conditions. The value \( m_1 = 1 \) in the recurrence relation yields

\[
\frac{d(m_2)}{\sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}}} + \frac{d(1)}{\sqrt{1 + \frac{1}{2} m^{-1}} - \sqrt{1 - \frac{1}{2} m^{-1}}}
\]
(using $t_{0,m_2,m_3+1} = 0$) which allows us to determine $t_{2,m_2,m_3+1}$ uniquely. All other values of $t$ for $m_1 > 2$ are fixed in the same way, and a similar analysis holds for varying $m_2$. This shows that we need to specify the values

$$t_{1,m_2,m_3} \text{ and } t_{m_1,1,m_3} \text{ for all } m_1, m_2, m_3 > 0$$

(29)
as boundary data together with initial values at fixed $m_3$.

As for the initial values, one would expect to need the wave function at two slices of constant $m_3$ because the evolution equation is of second order. However, by definition $t_{m_1,m_2,m_3}$ has to vanish for $m_3 = 0$ which is equivalent to the fact that $s_{n_1,n_2,0}$ drops out of the evolution equation. Thus, arbitrary initial values at fixed $m_3^{(0)}$ and $m_3^{(0)} + 1$ will not be consistent with this condition and the evolution to $m_3 = 0$ will yield linear relations for the initial data. Consequently, only the values at one slice of fixed $m_3^{(0)}$ are free and the number of initial conditions is only half the expected amount, as in the isotropic case. Unlike the isotropic situation, however, this does not suffice to specify the gravitational part of the wave function uniquely up to norm. Further conditions can be expected to arise from the requirement of a pre-classical wave function at large volume \[4\] where the wave function should not oscillate on Planck scales. This also restricts the original wave function $s_{n_1,n_2,n_3}$ at odd values of $n_1$, which are not determined by $t_{m_1,m_2,m_3}$. Such an analysis, however, is more complicated for a partial difference equation and will be pursued elsewhere. Figs. 1 and 2 show two different impressions of a solution to the Hamiltonian constraint of the Bianchi I LRS model which represents a wave packet moving through the classical singularity. Details of this model and its classical and Wheeler–DeWitt behavior, as well as more informations about the figures, can be found in the Appendix.

### 4.3 Flat Space-Time

It is usually hard to find exact solutions of a partial difference equation as (27) with non-constant coefficients, even if it is linear. In our case it is easy to see that $t_{m_1,m_2,m_3} = m_1$, $t_{m_1,m_2,m_3} = m_2$, and $t_{m_1,m_2,m_3} = m_3$ are exact solutions in the vacuum case. However, they do not satisfy the conditions (26) and thus are not allowed.

An approximate solution at large volume can be seen to be of the form $t_{m_1,m_2,m_3} = m_1m_2m_3$. It does fulfill the conditions (26), but this is not relevant since the solution is valid only approximately at large $m_1$, $m_2$, $m_3$. To see that this is an approximate solution we expand $d(m) = \frac{1}{2}m^{-1} + O(m^{-2})$ such that the left hand side of (27) becomes the constant 6 up to terms of the order $m^{-1}$. This corresponds to a negative matter energy density $\rho_{\text{matter}} \sim -6\gamma^{-3}\kappa^{-1}p^{-2}V^{-2}$ which decreases like the inverse second power of the volume and thus would be negligible compared to any other standard matter component at large volume. In fact, the solution $t_{m_1,m_2,m_3} = m_1m_2m_3$, which corresponds to $s_{n_1,n_2,n_3} \propto \text{sgn}(n_1n_2n_3)\sqrt{|n_1n_2n_3|} \propto \text{sgn}(n_1n_2n_3)V_{n_1,n_2,n_3}$, represents flat space in the sense that all terms in the constraint $c_1c_2a_3 + c_2c_3a_1 + c_3c_1a_3 = 0$ which follows from (7) vanish separately. At large volume a quantization of $a_3 = \sqrt{|p|p^2/p|} \text{sgn}(p^3)$ must have approximate eigenvalues of the form $\sqrt{|n_1n_2/n_3|} \text{sgn}(n_3)$ such that in the triad representation we
Figure 1: Contour lines for a wave packet of the Bianchi I LRS model moving through the classical singularity (the diagonal line where the wave function drops to zero). The lower right boundary corresponds to the boundary $m = 0$ of the minisuperspace, while the upper left boundary has been introduced for numerical purposes. (Not all values of the wave function are plotted; see the Appendix for further explanation.)

Figure 2: Closer look at the classical singularity. Lattice points are values of the discrete wave function $t_{mn}$. 
have for our approximate solution \((\hat{a}_3 s)_{n_1,n_2,n_3} \propto n_1 n_2\). In the connection representation, this corresponds to the state

\[
\hat{a}_3|s\rangle = \sum_{n_1,n_2,n_3} n_1 n_2 |n_1,n_2,n_3\rangle \propto \tilde{\delta}(c_1)\tilde{\delta}(c_2)\tilde{\theta}(c_3)
\]

where \(\tilde{\delta}(c) := \sum_j (2j+1)\chi_j(c)\) denotes the \(\delta\)-distribution on \(SU(2)\) and also \(\tilde{\theta}(c) := \sum_j \zeta_j(c)\) is to be interpreted in a distributional sense. Therefore, one would expect that \(\hat{a}_3|s\rangle\) is annihilated by a quantization of \(c\) as a multiplication operator, which appears in the constraint. However, as already seen, the annihilation is not complete which leads to the matter contribution decreasing as the inverse second power of the volume. To understand this fact we have to take into account that the configuration space (for a single diagonal component) differs from \(SU(2)\) precisely in the singularity structure of the point \(c = 0\) which is a fixed point of the gauge transformations. Correspondingly, the state space for a single diagonal component is not given simply by gauge invariant functions on \(SU(2)\), i.e., only the characters \(\chi_j\), but by all possible functions generated by \(\chi_j\) and \(\zeta_j\). Since \(\zeta_j\) is not regular in \(c = 0\) for any \(j\), an ordinary \(\delta\)-distribution on this space of states cannot be well-defined. Instead, the distribution \(\tilde{\delta}\) introduced above appears which can be regarded as a regularization of the ill-defined naive \(\delta\)-distribution.

For regular test functions \(f(c)\), \(\tilde{\delta}\) in fact has the expected action, as can be checked in the usual way:

\[
(2\pi)^{-1} \int \tilde{\delta}(c) f(c) \sin^2(\frac{1}{2}c) dc = (2\pi)^{-1} \sum_j \int (2j + 1) \sin((j + \frac{1}{2})c) \sin(\frac{1}{2}c) f(c) dc
\]

\[
= \pi^{-1} \sum_j \int_0^{4\pi} \cos((j + \frac{1}{2})c) \frac{d}{dc}(f(c) \sin(\frac{1}{2}c)) dc
\]

\[
= 2\pi^{-1} \sum_{n \in \mathbb{N}} \int_0^{2\pi} \cos(nc)(f'(2c) \sin c + \frac{1}{2}f(2c) \cos c) dc
\]

\[
= 2(f'(2c) \sin c + \frac{1}{2}f(2c) \cos c)|_{c=0} - \pi^{-1} \int_0^{2\pi} (f'(2c) \sin c + \frac{1}{2}f(2c) \cos c) dc
\]

\[
= f(0)
\]

where we used the \(U(1)\) \(\delta\)-distribution \(\delta(t) = (2\pi)^{-1} \sum_{n \in \mathbb{Z}} e^{int} = (2\pi)^{-1} (2 \sum_{n \in \mathbb{N}} \cos(nt) + 1)\) and periodicity of \(f\) and \(f'\). If \(f\) is not regular in \(c = 0\), however, i.e., of the form \(f(c) = g(c) \sin(\frac{1}{2}c)^{-1}\) with a periodic function \(g\) which is regular and non-zero in \(c = 0\), we have

\[
(2\pi)^{-1} \int \tilde{\delta}(c) f(c) \sin^2(\frac{1}{2}c) dc = (2\pi)^{-1} \sum_j \int (2j + 1) \sin((j + \frac{1}{2})c) g(c) dc
\]

\[
= 2\pi^{-1} \sum_{n \in \mathbb{N}} \int_0^{2\pi} \cos(nc)g'(c) dc = 2g'(0).
\]
Thus, the regularized $\delta$-distribution is

$$\tilde{\delta}[f] = 2\frac{d}{dc}\left(\sin\left(\frac{1}{2}c\right)f(c)\right)|_{c=0} = \begin{cases} f(0) & \text{if } f \text{ regular in } c = 0 \\ 2g'(0) & \text{if } f(c) = g(c)\sin\left(\frac{1}{2}c\right)^{-1} \end{cases} . \quad (30)$$

Since the $\delta$-distribution is regularized in order to take into account non-regular test functions, it is not annihilated when multiplying with $\sin\left(\frac{1}{2}c\right)$ or $c$. Instead, we have

$$(2\pi)^{-1}\int\sin\left(\frac{1}{2}c\right)\tilde{\delta}(c)f(c)\sin^2\left(\frac{1}{2}c\right)dc = 2\pi^{-1}\int_0^{2\pi} \sum_{n \in \mathbb{N}} \cos(nc)(f'(2c)\sin^2 c + f(2c)\sin c\cos c)dc$$

$$= 0 \quad \text{if } f \text{ regular}$$

but

$$(2\pi)^{-1}\int\sin\left(\frac{1}{2}c\right)\tilde{\delta}(c)f(c)\sin^2\left(\frac{1}{2}c\right)dc = (2\pi)^{-1}\int \tilde{\delta}(c)g(c)\sin^2\left(\frac{1}{2}c\right)dc$$

$$= g(0) \quad \text{otherwise.}$$

In fact, it is easy to check that we obtain the distribution $\tilde{0}$ defined above when we multiply with $\sin\left(\frac{1}{2}c\right)$:

$$\tilde{0}[f] = (2\pi)^{-1}\int \tilde{0}(c)f(c)\sin^2\left(\frac{1}{2}c\right)dc = (2\pi)^{-1}\sum_{n \in \mathbb{N}} \int \cos\left(\frac{1}{2}nc\right)f(c)\sin\left(\frac{1}{2}c\right)dc$$

$$= (f(2c)\sin c)|_{c=0} = \begin{cases} 0 & \text{if } f \text{ regular} \\ g(0) & \text{if } f(c) = g(c)\sin\left(\frac{1}{2}c\right)^{-1} \end{cases} .$$

Thus, $\sin\left(\frac{1}{2}c\right)\tilde{\delta} = \tilde{0}$ and we have to multiply a second time to get zero, $\sin\left(\frac{1}{2}c\right)\tilde{0} = 0$.

In the isotropic model we have the same structure of the singularity $c = 0$ in the configuration space, but there the constraint is quadratic in the single gauge invariant connection component $c$ which annihilates the regularized $\delta$-distribution. Therefore, there is no remaining matter contribution in the isotropic case. This demonstrates how certain features of a theory can be lost when additional symmetries are introduced, and also that working with gauge-invariant $SU(2)$-states (11) and (12) can lead to results different from those obtained with $U(1)$-states $e^{inc}$ which would appear in a gauge-fixed theory. In this example, however, the physical relevance is not clear. Furthermore, it is an effect of the singularity structure in $c_I = 0$ which we can probe here since we are looking for solutions of flat space-time which are $c_I = 0$ classically. For other solutions the set $c_I = 0$, which is of measure zero in the minisuperspace, is not expected to contribute significantly. However, such solutions corresponding to the classical Kasner behavior are harder to find even approximately, and one has to resort to a numerical analysis. Some difficulties to be faced are discussed in the Appendix.
5 Discussion

In this paper we developed loop quantum cosmological techniques for homogeneous cosmological models. The calculations have been simplified considerably by diagonalizing the canonical degrees of freedom, a process which retains all the relevant physical information. Most importantly, the volume operator is simpler and it is possible to find its spectrum explicitly. Having a simple volume operator then also leads to explicit expressions such as inverse metric operators and the Hamiltonian constraint operator which are necessary to study the classical singularity. Extending the results for isotropic models, we now have practical techniques for a larger class of systems given by all Bianchi class A models and their locally rotationally symmetric submodels (which have a single rotational axis). Those models are dynamically non-trivial even in the vacuum case such that they allow us to study quantum geometry effects independently of the matter coupling.

Here we mainly applied the techniques to the Hamiltonian constraint of the Bianchi I model. It turned out that the classical singularity is absent in loop quantum cosmology in very much the same way as in the isotropic case. In particular, it is the same factor ordering of the constraint operator which is selected by the requirement of a non-singular evolution. New features compared to the isotropic case also emerged: it has been seen to be essential that quantum geometry is based on densitized triad variables, and the issue of initial conditions is more complex. One has to choose not just initial conditions but also boundary conditions on minisuperspace, and the issue of pre-classicality is more complicated to analyze. It may turn out that pre-classical wave functions (up to norm) fulfilling the consistency conditions are not unique, but still the freedom is reduced compared to the Wheeler–DeWitt approach.

The analysis has also been simplified by choosing a diagonal component of the triad as internal time, rather than the volume. Even though the volume spectrum is known explicitly, its use as internal time would lead to a more complicated evolution equation since it is not equally spaced. For the Bianchi I model with its classical Kasner behavior, a diagonal component as internal time is justified, and it is well suited to study the approach to the classical singularity. In other Bianchi models the behavior is certainly more complicated: one expects a succession of different Kasner epochs. While in all those epochs the triad components $p^I$ are all decreasing toward the singularity, it is not always clear what happens during transitions between different epochs. If the behavior of the triad components remains monotonic during the transitions, one can use one of them as internal time and follow the evolution. Note that the result of an absence of a singularity will hold true in any case since it is a statement about the possibility of extending the wave function throughout all of minisuperspace uniquely; choosing an internal time is then only necessary to develop an evolution picture.

Particularly interesting is the Bianchi IX model which has been suspected to behave chaotically. Here one can check if the modified approach to classical singularities in quantum geometry, which has been observed in the isotropic case in [5] and been seen to lead to inflation, implies a different behavior. In isotropic models, the origin of a modified approach comes from quantum geometry effects in the matter Hamiltonian while the grav-
The computational part of the effective classical constraint equation has been left unmodified in a first approximation. In Bianchi models other than type I one expects a similar modification even in the vacuum case because the spin connection is non-zero and depends on triad components. This has to be dealt with properly when quantizing the Hamiltonian constraint and opens the door for modifications in effective classical equations of motion. While this does not modify the kinetic part (i.e., the terms containing time derivatives in Equation 8) of the Hamiltonian constraint in a first approximation, it leads to a modified potential containing the spin connection at small volume. One can then expect that the series of transitions between Kasner epochs, which can be seen as reflections of the scale factors on the potential well, will change since the potential well breaks down if the volume is small enough. This may stop the reflections altogether and lead to a non-chaotic behavior. Then, a single Kasner epoch would be responsible for the transition through the classical singularity, which would not look much different from the Bianchi I behavior close to the singularity. These issues will be discussed in more detail elsewhere.

The Bianchi IX model also provides further clues for the full theory. It has been speculated that the approach to inhomogeneous singularities is described by the BKL scenario according to which different points on a space-like slice decouple from each other close to a singularity (technically, only time derivatives remain in an asymptotic expansion of Einstein’s equations close to a singularity). If this scenario is true and can be used in the quantum theory, it suggests that a non-singular Bianchi IX behavior implies non-singular behavior in the full theory. However, since even the classical validity of the BKL scenario is far from being established, such a conclusion would be premature at present.

An alternative route is to study less symmetric models and see if what we have learned from more symmetric ones remains true. In this paper we presented the first step, going from isotropic models to anisotropic but still homogeneous ones. It turned out that essential results did not change, in particular the evolution remains non-singular. Even though the mechanism is similar to that in isotropic models, there are non-trivial aspects which cannot be seen in an isotropic model. It could well have happened that there is a singularity in homogeneous models but not in isotropic ones, e.g., if one used a theory based on the co-triad rather than the densitized triad as fundamental variable. That quantum geometry so far has provided precisely those properties one would need to have non-singular behavior is encouraging, but it also indicates that there may still be further surprises when we go one step further by studying inhomogeneous midisuperspace models.

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Appendix

A  The Bianchi I LRS Model

Probably the most simple anisotropic model is the Bianchi I LRS model without matter, which is defined as the subclass of Bianchi I geometries admitting one spatial rotational symmetry axis. Therefore, two of the diagonal components of the connection as well as of the triad, e.g. the first two for definitiveness, have to equal each other and only two degrees of freedom are left which we choose to be \((c, p_c)\) and \((A, p_A)\) embedded into the Bianchi I model by

\[(A, c) \mapsto (c_1, c_2, c_3) = (A, A, c) \quad \text{and} \quad (p_A, p_c) \mapsto (p^1, p^2, p^3) = (p_A, p_A, p_c).\]

The symplectic structure derived from the embedding follows from (3):

\[\{A, p_A\} = \frac{1}{2} \gamma \kappa, \quad \{c, p_c\} = \gamma \kappa.\]

For the LRS model the constraint (7) reduces to

\[H = -2\gamma^{-2}\kappa^{-1}|p_c|^{-\frac{3}{2}}A(2cp_c + Ap_A) \propto Ap_A + 2cp_c\]

which implies the equations of motion

\[\dot{p}_A = \frac{1}{2}p_A, \quad \dot{A} = -\frac{1}{2}A, \quad \dot{p}_c = 2p_c, \quad \dot{c} = -2c\]

solved by

\[p_A(\tau) \propto \sqrt{\tau}, \quad A(\tau) \propto \tau^{-\frac{1}{2}}, \quad p_c(\tau) \propto \tau^2, \quad c(\tau) \propto \tau^{-2}.\]

Using \(p_c\) as internal time we can write the evolution of \(p_A\) as \(p_A(p_c) \propto p_c^{\frac{1}{2}}\), which coincides with the Kasner behavior restricted to the LRS case: If two of the Kasner coefficients are equal, we have \(2\alpha_1 + \alpha_3 = 1 = 2\alpha_1^2 + \alpha_3^2\) implying \(\alpha_1 = \frac{2}{3}\) and \(\alpha_3 = -\frac{1}{3}\). In the Kasner time coordinate \(t\) we then have \(p_A \propto t^\frac{1}{4}\), \(p_c \propto t^\frac{3}{4}\) according to (11), which also leads to \(p_A(p_c) \propto p_c^{\frac{1}{2}}\).

The Wheeler–DeWitt equation in the triad representation for the Hamiltonian \(Ap_A + 2cp_c\) can be written in the form

\[\left(\frac{1}{2}p_c^{-1} \frac{\partial}{\partial p_A} p_A + 2 \frac{\partial}{\partial p_c}\right) \tilde{\psi}(p_A, p_c) = 0\]

where a factor of \(p_c\) has been absorbed in the wave function \(\tilde{\psi}(p_A, p_c) := p_c\psi(p_A, p_c)\). Fig. 3 shows a solution which represents a wave packet following the classical trajectory \(p_A(p_c) \propto p_c^{\frac{1}{2}}\) in minisuperspace, hitting the classical singularity.

In the loop quantization we have only two integer labels \(m\) and \(n\), where \(m\) represents the value of the two equal triad components \(p_A\) and \(n\) the third one, \(p_c\). Residual gauge
Figure 3: A solution to the Wheeler–DeWitt equation of the Bianchi I LRS model. When the wave packet approaches the classical singularity (upper right corner), its amplitude diverges. The minisuperspace boundary $p_A = 0$ is at the right.

Transformations can now be seen to change the sign of $m$ such that we can get unique representatives of gauge equivalence classes by considering only non-negative values of $m$. The label $n$, on the other hand, is allowed to take any integer value and thus is best suited to describe the transition through the classical singularity. We will use it as internal time, the sign of which, $\text{sgn}(n)$, is again the orientation.

For the sake of simplicity we write down directly the evolution equation for a wave function $t_{m,n}$ in the form (27) which now becomes

$$
2d_2(m)(t_{n+1,m+1} - t_{n+1,m-1}) + d(n)(t_{n,m-2} - 2t_{n,m} + t_{n,m+2})
+2d_2(m)(t_{n-1,m-1} - t_{n-1,m+1})
= 2d_2(m)\tilde{t}_{n+1,m} + d(n)(\tilde{t}_{n,m+1} - \tilde{t}_{n,m-1}) - 2d_2(m)\tilde{t}_{n-1,m} = 0.
$$

Here, we defined $\tilde{t}_{n,m} := t_{n,m+1} - t_{n,m-1}$ and $d_2(m) := m^{-1}$ for $m \neq 0$ and $d_2(0) := 0$ (it replaces $d(m)$ of (25) since now two labels in the volume eigenvalues are equal to each other).

We now have the evolution equation in the form of a partial difference equation in two independent variables, which is straightforward to implement numerically. It is, however, a non-trivial problem to find numerical solutions which are close to pre-classical ones, i.e., which vary significantly only on large scales. We have many parameters for a solution, initial values at one $n$-slice and boundary values at small $m$. To find a solution which satisfies the consistency condition ($\tilde{t}_{0,m} = 0$), we can choose the initial values at the $n$-slice
and the boundary values freely. A complete initial value problem would be specified by also choosing values at the next \( n \)-slice since the evolution equation is of second order in \( n \). We can find the values of the second slice by first leaving them as free parameters, solving the evolution equation up to \( n = 0 \) where we obtain \( \tilde{t}_{0,m} \) as linear functions of the free initial values, and solving the set of linear equations \( \tilde{t}_{0,m} = 0 \). The result is a solution which by construction satisfies the consistency condition. In practice, we have to face the following problems when we want to find a numerical solution which is also pre-classical:

- There is no guarantee that the computed consistent initial data at the second \( n \)-slice are close to the ones chosen at the first slice (which would be necessary for pre-classicality). One can try to find such a solution by picking appropriate initial and boundary values, but it is complicated by the large amount of initial and boundary parameters we have to choose.

- For numerical purposes we have to introduce a second boundary at large \( m \), which can introduce artificial boundary effects.

- The initial values should represent a pre-classical function such that differences appearing in the evolution equation are small. This requires a large lattice in the \( m \)-direction which increases the numerical effort to evolve and to solve the system of linear equations in order to find the initial values at the second \( n \)-slice. Furthermore, more \( m \)-values increase the likelihood of rounding errors adding up.

- Close to classical singularities the wave packet can move rapidly on the lattice (corresponding to large extrinsic curvature). If this happens even between two consecutive \( n \)-slices, differences in the \( n \)-direction will become large which can lead to contributions increasing exponentially toward the classical singularity. While imposing the consistency conditions exactly would eliminate those contributions, they will always be present in a numerical analysis and can even lead to wrong initial values due to rounding errors.

In order to show an illustration of a possible pre-classical solution, Figs. 1 and 2 have been obtained as follows: First, the evolution equation shows that for large \( n \) we have \( \tilde{t}_{n+1,m} \approx \tilde{t}_{n-1,m} \), provided that the \( m \)-differences of \( \tilde{t} \) are small. Therefore, we can suppress possible oscillations in the \( n \)-direction, coming from consistent initial values at the second \( n \)-slice not close to the one on the first slice, by plotting only every second \( n \)-value. Secondly, in order to avoid a rapid movement of the wave packet in the \( m \)-direction, the lattice has been stretched in the \( n \)-direction by using the Hamiltonian \( H_k = A p_A + 2 k c p_c \). While the original value \( k = 1 \) leads to a rapid movement at small \( n \) which implies rounding errors due to exponentially increasing contributions and an unacceptable numerical solution, this turns out not to pose a problem for \( k \geq 4 \) (\( k = 4 \) in the figures) since the movement would happen between \( n = 0 \) and \( n = 1 \) which is not visible.

One could think that it is even impossible to find a pre-classical wave function reflecting the fact that DeWitt’s initial condition, which is close to the result of the dynamical initial
condition, is ill-posed in this model (i.e., its only solution would be zero). This, however, is not the case for two reasons: first, the notion of pre-classicality allows some tolerance since a discrete wave function can only be required to be close to a smooth one, but not exactly smooth; and secondly, the discreteness leads to a different behavior of solutions at small $n$ such that a DeWitt-like initial condition is in fact well-posed (see [11]).

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