Loop quantum cosmology: IV. Discrete time evolution

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Abstract
Using general features of recent quantizations of the Hamiltonian constraint in loop quantum gravity and loop quantum cosmology, a dynamical interpretation of the constraint equation as evolution equation is presented. This involves a transformation from the connection to a dreibein representation and the selection of an internal time variable. Due to the discrete nature of geometrical quantities in loop quantum gravity, time also turns out to be discrete leading to a difference rather than differential evolution equation. Furthermore, evolving observables are discussed within this framework, which enables an investigation of physical spectra of geometrical quantities. In particular, the physical volume spectrum is proven to equal the discrete kinematical volume spectrum in loop quantum cosmology.

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1. Introduction

One of the major open issues of loop quantum gravity [1] is to understand its dynamics which is governed by the Wheeler–DeWitt equation. However, this equation in the full theory (e.g. [2]) contains all the complicated details of the evolution and is plagued not only by technical problems but also by conceptual issues, most importantly the problem of time. At this point, reductions to simpler but still representative models may be helpful, a strategy which in previous approaches to (quantum) gravity has been widely used. Dynamical issues are most conveniently studied in cosmological models which are obtained by a reduction of gravity to homogeneous geometries. For loop quantum gravity, this reduction has been performed in [3] by specializing the general symmetry reduction scheme for diffeomorphism-invariant quantum theories of connections [4]. Within this framework we have already derived quantizations of the Hamiltonian constraint for various models [5] which will now be used to investigate the dynamics governed by those operators.

The study of (quantum) cosmological models has been initiated in order to understand the very early stages of the universe and to gain insights which can also be used in the full
theory. With the lack of a complete quantum theory of gravity, however, the only route to quantum cosmology has been to perform a quantization after the classical symmetry reduction (minisuperspace quantization [6, 7]). Although it is not at all clear, and can from this perspective not be decided, whether the immense restriction to finitely many degrees of freedom is mild enough to maintain typical properties of full quantum gravity, minisuperspace models provide interesting test-beds for problems of quantum gravity. Due to their finite number of degrees of freedom they are quantum mechanical models, but their dynamics is, as it is inherited from the theory of general relativity, still intrinsic. This means that it is not governed by a Schrödinger equation for the evolution of a wavefunction in an external time parameter, but by the Wheeler–DeWitt equation which is a constraint equation expressed solely in terms of the metrical variables and their conjugate momenta corresponding to the fact that the theory is invariant under arbitrary reparametrizations of time. At first sight, there seems to be no dynamics at all in this constraint formulation, which leads to the name ‘frozen time formalism’.

In order to interpret the Wheeler–DeWitt equation as a time evolution equation one has to introduce an internal time which is constructed from metrical or matter degrees of freedom (see, e.g., [8] and references therein). In a homogeneous context one usually chooses the scale factor of the universe (related to the determinant of the metric), in which the Wheeler–DeWitt equation is a hyperbolic differential equation of second order (this also holds true after introducing inhomogeneous perturbations [9]).

Let us illustrate these considerations with simple examples. In an isotropic flat model, in which space looks the same not only at all points but also in all directions, the only metrical degree of freedom is described by the scale factor \(a\) appearing in the spatially isotropic metric 
\[
\mathrm{d}s^2 = -\mathrm{d}t^2 + a(t)^2(\mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2).
\]
A model with only one degree of freedom can, in a formalism without extrinsic time, not exhibit any dynamics: there simply is nothing to build a clock. In the spacetime picture this corresponds to the fact that the classical solutions are maximally symmetric (not only in space but in spacetime): Minkowski space for a vanishing cosmological constant or de Sitter/anti-de Sitter space. The simplest matter field which can be coupled is an isotropic scalar field \(\phi\). We now have two degrees of freedom, \(a\) and \(\phi\), and dynamics which is usually written down in terms of Lagrangian or Hamiltonian equations of motion. Although these equations are differential equations for \(a(t)\) and \(\phi(t)\) in terms of a time parameter \(t\), this parameter can be reparametrized (gauged) arbitrarily. In this simple model one can immediately remove \(t\) in order to arrive at an intrinsic time formalism: from the differential equations for \(a(t)\) and \(\phi(t)\) one can obtain a differential equation for \(\phi(a)\), where \(a\) is regarded as intrinsic time. Its solution describes the evolution of the scalar field \(\phi\) in an expanding or contracting branch of the universe and contains all invariant information about the model. In a more complicated situation one can, similarly, make sense only of relational motions of degrees of freedom with respect to each other, and not with respect to an external time. Analogously, in a minisuperspace quantization we can describe the states by wavefunctions \(\psi(a, \phi)\) (often dubbed the ‘wavefunction of the Universe’) subject to the Wheeler–DeWitt equation \(\hat{H}\psi = 0\). Here, no external time parameter appears from the outset, and the information contained in \(\psi(a, \phi)\) is relational: interpreted as a probability density, it describes the possible values of \(\phi\) in relation to the values of \(a\).

Other widely used cosmological models are the Bianchi models, which describe homogeneous, but not necessarily isotropic, geometries. Therefore, the metric is parametrized by more than one degree of freedom, and one can study the dynamics of the vacuum solutions without coupling matter fields. This has been done in [10] with the following basic results. The metric can be consistently diagonalized (in some models this is just a gauge fixing, whereas in others it is a further truncation in addition to the symmetry requirement [11]) such that there
are only three coordinates usually denoted as $\beta^0$ (the scale factor) and $\beta^1, \beta^2$ (the anisotropies) and their canonically conjugate momenta $\pi_0, \pi_1, \pi_2$. In a suitable gauge which also specifies the lapse function the Hamiltonian is given by

$$\mathcal{H} = \frac{1}{2} \eta^{ij} \pi_i \pi_j + V(\beta^I) \approx 0$$

where $\eta$ is a constant metric on minisuperspace with signature $(-, +, +)$ and $V$ is a potential which characterizes the specific Bianchi model. For Bianchi I the potential $V$ vanishes, which can also be achieved for other models after suitable coordinate transformations on minisuperspace, and the Hamiltonian consists of just the ‘kinetic’ term containing the momenta.

In the quantum theory of this model we can choose the $\beta$-representation in which wavefunctions $\psi$ depend on the parameters $\beta^I$, i.e. they are functions on minisuperspace. As usual, the momenta are then represented as derivative operators and the Wheeler–DeWitt equation takes the form

$$\frac{1}{2} \eta^{ij} \frac{\partial^2}{\partial \beta^i \partial \beta^j} \psi(\beta) = 0$$

of a Klein–Gordon equation where $\beta^0$, again the scale factor, plays the role of time. An interpretation as an evolution equation in the intrinsic time $\beta^0$ is then immediate. However, we can just as well choose a $\pi$-representation by using wavefunctions which depend on the momenta. In this case, the Wheeler–DeWitt operator would not be a derivative but a multiplication operator, and the Wheeler–DeWitt equation would not have an interpretation as an evolution equation but instead constrain the support of wavefunctions. Of course, both pictures are equivalent, as in usual quantum mechanics, but we see that the emergence of an evolution equation depends on the representation once an internal time is selected. This issue is characteristic for a generally covariant model where the internal time is to be found under the internal degrees of freedom, which do not have a unique representation.

There is an important lesson we have to learn from these considerations. In cosmological scenarios it is most convenient to choose the scale factor as a time variable (although this was the case in both examples, the selection of an internal time is by no means unique; furthermore, in more complicated models, let alone the full theory, there are no explicitly known time functionals) and to study the evolution of other degrees of freedom (matter or metrical) with respect to this parameter. In a minisuperspace quantization one then has to use a metric representation in order to extract an evolution equation. Using metrical variables $(q_{ab}, p^{ab})$ this is the usual representation anyway, but the largest successes with respect to kinematical aspects of quantization have been achieved in loop quantum gravity using connection variables where one bases the quantum theory on the connection (or loop) representation. Also the quantum symmetry reduction to homogeneous models [3] leads at first to a connection representation such that, afterwards, we have to transform to a dreibein representation and find an interpretation of the Wheeler–DeWitt equation as an evolution equation. Here, one can expect significant departures from the usual minisuperspace quantizations described above, because the volume, which has been used as an internal time, is now quantized at least at the kinematical level [12, 13] (note that the parameters $a$ and $\beta^0$ above can take all positive values and thus show no volume quantization). We will see that this implies a discrete time and a difference (not differential) equation as an evolution equation.

Our strategy [14] is the following: using [3] we perform the symmetry reduction for the above models at the kinematical level of loop quantum gravity by selecting homogeneous states. Alternatively, the procedure can be interpreted as a loop quantization of minisuperspaces. As

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2 The author is grateful to A Ashtekar for this suggestion.
shown in [15], this leads to discrete geometric spectra after the symmetry reduction, whereas a usual minisuperspace quantization after a classical symmetry reduction leads to a continuous volume spectrum. The dynamics of our models is governed by the Hamiltonian constraint operators which have been derived in [5] and will be recalled briefly in the following section. In the main part of this paper we will perform the transformation into a dreibein representation and discuss our interpretation of the constraint equation as an evolution equation. Finally, having an evolution equation, we can study evolving observables and will, in particular, show that the physical volume spectrum (taking into account the Hamiltonian constraint) equals the kinematical one (ignoring the Hamiltonian constraint).

2. Wheeler–DeWitt operators

We will first recall the loop quantum theory of homogeneous minisuperspaces derived in [3] and the Hamiltonian constraint operators of those models [5] which will be used in the remaining part of this paper. Because of their homogeneity the values of all fields in a single point suffice to completely characterize the spatially homogeneous canonical fields, namely the scalars \( \phi_i^I \tau_i \in L SU(2) \), \( 1 \leq I \leq 3 \) which determine a homogeneous connection \( A_I^a \tau_i = \phi_i^I \tau_i \omega_I^a \) in terms of invariant (with respect to the symmetry group) 1-forms \( \omega_I^a \) on \( \Sigma \) and their canonically conjugate momenta \( p_I^i \) which are derived from the dreibein components and, therefore, encode the degrees of freedom of the metric on \( \Sigma \). Consequently, a reduced formulation can be formulated in a single point rather than by fields on a space manifold \( \Sigma \) which explicitly shows the reduction to finitely many degrees of freedom. This also demonstrates that usual loop variables cannot be used to build an auxiliary Hilbert space because they would necessarily break the symmetry. Instead, one uses point holonomies which are \( SU(2) \)-elements associated with a single point and serve to describe quantum scalar fields. For Bianchi models (because we will use a Hamiltonian formulation we have to restrict our considerations to class A models whose structure constants \( c^{IF}_{IJ} \) fulfill \( c^{IF}_{IJ} = 0 \)) there are three independent point holonomies \( h_I \in SU(2) \), \( 1 \leq I \leq 3 \) (due to anisotropy) and quantum states are gauge-invariant functions (where the \( SU(2) \)-gauge group acts by joint conjugation of all three-point holonomies) of these three group elements. The behaviour under conjugation shows that a point holonomy can be represented as an ordinary holonomy associated with a closed loop embedded in an auxiliary manifold, and quantum states can be expanded in spin network states on graphs with three closed edges \( e_I \) meeting in a 6-vertex. We are then able to compare results derived for minisuperspaces with those of the full theory by restricting the latter to spin networks with a single 6-vertex. For instance, the volume operator for Bianchi models [15] is identical to the action on a 6-vertex of the volume operator in the full theory derived in [13] (but differs from that of [12], see also [16]).

For locally rotationally symmetric (LRS) or isotropic models, the three-point holonomies are no longer independent, but are related by the equations

\[
h(\rho(f)(e_I)) = Ad_{\lambda(f)} h(e_I)
\]

where \( f \) is an element of the isotropy group acting on the edges \( e_I \) via the representation \( \rho \), and \( \lambda \) is a homomorphism from the isotropy group to the gauge group \( SU(2) \) (see [3] for details). In particular, for isotropic models all three-point holonomies are related and quantum states can be expressed as functions on a single copy of \( SU(2) \). However, they are not ordinary spin network states on a single edge, but generalized spin network states which can have an insertion due to the gauge transformation on the right-hand side of equation (1). Details have been worked out in [15] where the volume operator has also been derived and diagonalized explicitly.
Finally, we will need the Hamiltonian constraint operators [5] which can be derived similarly to the full theory [2]. Adaptations in the regularization are necessary only because there is no continuum limit and because the reduced operators have to respect the symmetry. However, the splitting of the Lorentzian constraint in a Euclidean part and a potential term, and the usage of the extrinsic curvature can be adopted without changes. For Bianchi models the Euclidean constraint operator is

$$\hat{H}_E[N] = -4i(\iota' l_P^2)^{-1} N \sum_{IJK} \epsilon^{IJK} \text{tr} \left( h_I h_J h_K^{-1} h_{[I,J]}^{[I,K]} [h_K, \hat{V}] \right)$$

(2)

with the Planck length $l_P$ and $\iota' = \iota V_0^{-1}$ being related to the Immirzi parameter $\iota$ and the volume $V_0$ of space in a fiducial homogeneous metric. Furthermore, $h_I$ are point holonomies acting as multiplication operators using the definition

$$h_{[I,J]} := \prod_{K=1}^3 (h_K)^{\epsilon_{IJK}},$$

and $\hat{V}$ is the volume operator for Bianchi models.

Using the quantized extrinsic curvature [2]

$$\hat{K} = i\hbar^{-1} [\hat{V}, \hat{H}_E[N]]$$

the complete Lorentzian constraint can be written as

$$\hat{H}[N] = 8i(1 + \iota^2)(l_P^2)^{-1} V_0 N \epsilon^{IJK} \text{tr} \left( [h_I, \hat{K}][h_J, \hat{K}][h_K, \hat{V}] \right) - \hat{H}_E[N].$$

(3)

Constraint operators for LRS and isotropic models can be derived by inserting the conditions (1) into the operators for Bianchi models and evaluating the action on the reduced Hilbert spaces.

3. Dynamics

Following the usual procedure for interpreting the Wheeler–DeWitt equation of cosmological models as an evolution equation, we will now first transform to a dreibein representation and then introduce an internal time. This will allow us to demonstrate that the Hamiltonian constraint equation can be written as an evolution equation with discrete time.

3.1. Dreibein representation

In most discussions of loop quantum gravity one always works in the connection representation where quantum states are represented as functions on the space of connections which are usually expanded as linear combinations of spin network states. Also the Hamiltonian constraint has been quantized to an operator acting on this space of functions where the holonomies, which constitute the main part of the constraint operator, act as multiplication operators [2, 5]. Thus imposing the Wheeler–DeWitt equation will result in a restriction of the support of physical states being in the kernel of the quantum constraint. This is similar to the discussion recalled in the introduction of the standard minisuperspace quantization of the Bianchi I model, where the Wheeler–DeWitt equation in the $\pi$-representation restricts the support of wavefunctions. Note that the variables $\pi_I$ there are conjugate to the metrical variables which are also the connection variables in the present framework. As suggested in this context, formulated in a metric (or dreibein) representation the Wheeler–DeWitt equation usually allows an interpretation as an evolution equation which motivates the following discussion.
In a dreibein representation quantum states are represented as functions on the space of dreibein components. Whereas for the homogeneous models which are of interest here this space is finite-dimensional, in the full theory it is infinite-dimensional and a mathematical formulation on the relevant function spaces has to be done with great care. Up to now we always took the attitude that all our constructions in the reduced models should be as close to the full theory as possible, and using a technique which cannot be generalized to the infinite-dimensional space of the full theory would obviously spoil this aim. A rigorous formulation of the connection representation has been achieved by applying the theory of representations of $C^*$-algebras to a particular $C^*$-algebra constructed from holonomies. A similar procedure is not applicable for a dreibein representation and, whereas the space of connections could be compactified to the quantum configuration space $\mathcal{A}$ of the connection representation, a suitable compactification of the space of dreibein components is not obvious and, even worse, not reasonable from the physical point of view. Furthermore, the compactness of the space $\mathcal{A}$ means that in a quantum theory the conjugate momenta, i.e. the dreibein components, can have only discrete values, which we have already seen in the discrete spectra of geometrical observables (the dreibein components are quantized to angular momentum operators). Thus the quantum configuration space in a dreibein representation will be a discrete space.

We will follow here a strategy which makes use of the already known and mathematically well founded connection representation by constructing a transform from this representation to another representation which will be equivalent to a dreibein representation. As is well known from quantum mechanics, such a transform can be constructed by expanding a state in a given representation in terms of eigenstates of a complete set of commuting operators. In our case, these operators should be quantizations of the dreibein components or, in order to maintain gauge invariance, of the products $p_i^I p_{ji}^J$ which correspond to the metric components $g_{IJ}$. A more convenient procedure is to expand a state in the connection representation in spin network states (which are usually chosen as a basis, anyway) and to use the spins and vertex contractors (which can also represented by spins) as discrete coordinates of the ‘quantum dreibein space’. Obviously, all the spins (in the full theory we would have to include other discrete labels, e.g. knot invariants, parametrizing the diffeomorphism equivalence classes of graphs) form a complete set characterizing a state completely, and this description is equivalent to a dreibein or metric representation because all eigenvalues of metric components can be expressed in terms of the spins, and vice versa.

Introducing a model-dependent index set $\mathcal{I}$ which contains all allowed multi-labels $L$, we can write the decomposition of an arbitrary state $f$ in the connection representation as

$$f(A) = \sum_{L \in \mathcal{I}} f_L T_L(A)$$

(4)

where $\{T_L : L \in \mathcal{I}\}$ is an orthonormalized set of spin network states associated with the multi-labels $L$. For the Bianchi models we have

$$\mathcal{I}_{\text{Bianchi}} = \{L = (j_1, j_2, j_3, k_1, k_2, k_3) : j_i, k_I \in \frac{1}{2}\mathbb{N}_0\}$$

if we parametrize the 6-vertex contractor by the three spins $k_I$ ($j_i$ are spins associated with the external edges of the point holonomies). For LRS models we have two external edges, a contractor parametrized by a single spin $k$, and an additional label $i$ describing the insertion; for isotropic models there is only one spin $j$ and an insertion-label $i$ taking only two possible values [15]:

$$\mathcal{I}_{\text{LRS}} = \{(j_1, j_2, k, i)\}, \quad \mathcal{I}_{\text{iso}} = \{(j, i) : j \in \frac{1}{2}\mathbb{N}_0 \cup \{-\frac{1}{2}\}, i \in \{0, 1\}\}.$$ 

From now on we will call a state $f$ represented by the coefficients $f_L$ in the above expansion a state in the dreibein representation. In this representation states are maps $f : \mathcal{I} \to \mathbb{C}, L \mapsto f_L$. 


from the index set of the respective model to the complex numbers. The inner product can be derived from that in the connection representation (the Ashtekar–Lewandowski inner product): because the spin network states $T_L$ in the expansion of $f(A)$ were assumed to be orthonormalized in the Ashtekar–Lewandowski measure, we have

$$
(f, g) = \sum_{L, L' \in \mathcal{I}} \mathcal{J}_L \mathcal{J}_{L'} \langle T_L, T_{L'} \rangle = \sum_{L \in \mathcal{I}} \mathcal{J}_L \mathcal{J}_L.
$$

(5)

Thus, the kinematical Hilbert space is represented in the dreibein representation as $\mathcal{H}_{\text{kin}} = \ell^2(\mathcal{I})$, the completion of the space of square-integrable sequences on the index set $\mathcal{I}$.

### 3.2. Internal time

A central ingredient for a dynamical interpretation of a generally covariant theory is to choose one combination of the degrees of freedom as an internal time. In standard quantizations of homogeneous minisuperspaces (and their classical counterparts) this is usually done by using the scale factor (related to the spatially constant determinant of the metric on $\Sigma$) of the universe [6]. Besides providing the intuition that time is related to the expansion (or contraction) of the universe, this has the virtue of resulting in a hyperbolic differential equation (Wheeler–DeWitt equation) governing the evolution by means of a well posed initial-value problem.

In principle, we could copy this procedure and try to extract some interpretation of time from the volume spectrum in our quantizations of homogeneous models. However, the volume spectrum is, in general, quite complicated and not known explicitly for the Bianchi and LRS models. Although we know the volume spectrum for isotropic models [15], these models have only a single gravitational degree of freedom and we have to couple matter in order to obtain a reasonable dynamical system.

We therefore look for an acceptable substitute of the volume as internal time which we will motivate by using the classical Bianchi I model on $\mathbb{R}^3$. Its solutions, the Kasner solutions [17], can be written as

$$
\text{d}s^2 = -\text{d}t^2 + t^{2a_1} \text{d}x_1^2 + t^{2a_2} \text{d}x_2^2 + t^{2a_3} \text{d}x_3^2
$$

where the parameters $a_i$ have to obey the relations $\sum_I a_I = \sum_I a^2_I = 1$, i.e. there is only one independent parameter. One can see that there are always two positive and one negative parameter, so that two directions of space are expanding and the third one is contracting in such a way that the volume increases monotonically (due to $\sum_I a_I = 1$). In other models this behaviour is also the generic one in certain time intervals, the so-called Kasner epochs, where, however, a transition between different epochs is possible. The Kasner behaviour demonstrates that we can expect each diagonal metric component $g^{II}$, describing the expansion or contraction of the $I$th direction, to be as good an internal time as the scale factor. In a standard minisuperspace quantization we would now have to show that we obtain a hyperbolic evolution equation with such an internal time, but here we are at first mainly interested in a simple spectrum of the time parameter.

Let us therefore pick the first metric component $p^1 I p^1 I$ as a tentative time for Bianchi models. It is readily quantized using the usual procedure for point holonomies [3, 18]:

$$
\hat{p}_I^1 \hat{p}^1 I = \frac{1}{2} \mathcal{I}_p^2 \left[ J^{|I|}_{(\text{L})}(h_I) + J^{|I|}_{(\text{R})}(h_I) \right]^2.
$$

In order to determine its spectrum, we have to choose a suitable parametrization of the contractor in the 6-vertex, which can be done by decomposing it into a combination of four 3-vertices, the contractors of which are unique up to a constant factor. We do this by contracting first each of the closed external edges carrying spins $j_I$ to an internal edge carrying spin $k_I$;
the internal edges are then contracted in a central 3-vertex. We orient the edges in such a way that the internal ones are incoming in the central vertex, whereas the external edges have an incoming and an outgoing part in the three non-central vertices. All four 3-vertices are gauge invariant so that we have the relations
\[ J^{(L)}_i (h_1) - J^{(R)}_i (h_1) = L^{(L)}_i (1) \]
defining \( L^{(L)}_i (1) \) as a left-invariant angular momentum operator associated with the \( I \)th internal edge.

The computation of the spectrum of the diagonal metric components is now similar to that of the area spectrum (and to computations of spectra of coupled angular momenta):
\[ \hat{p}_i \hat{p}_i = \frac{1}{4} \ell^2 \pi^2 \left[ 2 J^{(L)}_i (h_1)^2 + 2 J^{(R)}_i (h_1)^2 - L^{(L)}_i (1)^2 \right] \]
immediately leads to the eigenvalues
\[ \frac{1}{4} \ell^2 \pi^2 \{4 j_1 (j_1 + 1) - k_1 (k_1 + 1) \} \].

We now have a candidate for an internal time with an explicitly known and simple spectrum, but we will even simplify this by using the external spin \( j_1 \) as a time label. Although we did not justify it as labelling eigenvalues of a quantization of a classically admissible time function, it is favourable because its lowest value, \( j_1 = 0 \), implies vanishing volume \( V = 0 \) (for a vanishing spin on one external edge the volume eigenvalues are those of a planar 4-vertex which always vanishes: there are only two independent angular momentum operators from which no non-vanishing antisymmetric product in three indices can be built). Ultimately, the justification of an internal time has to come from a reasonable interpretation of the dynamics as evolution in that degree of freedom, which will be studied below.

In other models, LRS or isotropic, we can similarly pick one of the labels of the quantum states as a candidate time label. We will, in general, decompose the label as \((n,L)\) where \( n \) is the time label and \( L \) denotes labels for all other remaining metric or matter degrees of freedom. For example, in Bianchi models, we have \( n = j_1 \) and \( L = \{j_2, j_3, k_1, k_2, k_3\} \), and in isotropic models \( n = j \) and \( L \) solely contains the insertion and possibly matter labels. Quantum states are then given in the dreibein representation by the coefficients \( c_{n,L} \), which is a discrete substitute of the wavefunction \( \psi(a,\phi) \) of standard minisuperspace quantizations.

The decomposition of the labels corresponds to a decomposition of the kinematical Hilbert space
\[ \mathcal{H}_{\text{kin}} = \ell^2 (I) = \bigoplus_n D_n \] into ‘equal-time’ subspaces \( D_n \) in which the time label \( n \) is fixed, but the remaining labels in \( L \) are arbitrary.

### 3.3. Discrete time evolution

After transforming to the dreibein representation and picking a candidate for an internal time, we are now ready to study the dynamics governed by the Wheeler–DeWitt operator (3). The essential part of this operator is the multiplication with a couple of holonomies, where the main contribution to the model dependence of the operator also enters.

In the connection representation the action of matrix elements of a holonomy \( h_{B}^{A} \) as a multiplication operator is given by
\[ h_{B_{0}...B_{j}}^{A_{0}...A_{j}} (h)^{A_{1}...A_{j}}_{B_{1}...B_{j}} = \pi \frac{\ell^2}{j} (h)^{A_{0}...A_{j}}_{B_{0}...B_{j}} \frac{2j}{2j + 1} \sum_{A_{j+1}...A_{2j}} h^{A_{j+1}...A_{2j}}_{B_{j+1}...B_{2j}} \epsilon_{A_{1}...A_{2j}} (B_{1}...B_{j}) \epsilon_{B_{1}...B_{j}} \]
where $\pi^j$ denotes the matrix representation of $SU(2)$ associated with spin $j$. This action can be transformed to the dreibein representation and written schematically as (acting on a state $c \in \ell^2(I)$)

$$(hc)_j = h_{j+\frac{1}{2}}c_j + h_{j-\frac{1}{2}}c_{j-\frac{1}{2}}$$

suppressing all but the one label associated with the edge underlying the holonomy $h$. Here, the coefficients $h_j$ are not just real numbers but operators acting on the subspaces of the kinematical Hilbert space with fixed $j$, i.e. in general they change the remaining labels which have been suppressed in the above equation. For example, in the Bianchi models, the external spins $j_I$, and therefore our internal time $n = j_1$, are changed only by multiplication with the holonomy $h_I$ associated with the same edge as the spin. However, the internal spins $k_I$ are affected by all holonomy multiplications because they parametrize the contractor which always is subject to change. Similarly, in LRS and isotropic models, external spins are changed only by multiplication with the appropriate holonomy, whereas the insertion and the contractor are changed by all holonomies.

From now on we will mainly be interested in the ‘time spin’ $n$ and the holonomy (denoted as $h_n$ in what follows) affecting it. Note that this is possible only because we selected a spin of an external edge as our internal time; otherwise the following considerations would be more complicated. Each $h_n$ appearing in the constraint operator leads to a combination of coefficients with labels $n + \frac{1}{2}$ and $n - \frac{1}{2}$ of a state in the dreibein representation. Because there is always more than one holonomy associated with a fixed edge in the constraint operator, we have in general an action of the form

$$(\hat{H}c)_n = \sum_{i=-\omega/2}^{\omega/2} (H_i c)_{n+i/2}$$

again suppressing the labels in $L$ and introducing the operators $H_i$ which fix each of the subspaces $D_n$. The number $\omega$ is defined as twice the maximal number of holonomies $h_n$ appearing in each summand of the constraint operator; it also determines the number of operators $H_i$ which is given by $\omega + 1$.

Because $\hat{H}$ is a quantized constraint operator, all physical states $s$ have to obey the Wheeler–DeWitt equation

$$\sum_{i=-\omega/2}^{\omega/2} (H_i s)_{n+i/2} = 0 \quad \text{for all } n \in \frac{1}{2}\mathbb{N}_0.$$  \hspace{1cm} (9)

In this form, recalling that $n$ is our internal time label, we can immediately read off a discrete evolution equation: the Wheeler–DeWitt equation is an implicit difference equation of generic order $\omega$ which, however, is reduced up to $\frac{1}{2}\omega$ for small $n$ because in the holonomy multiplication there is only one term when acting on the $n = 0$ state. Provided the highest-order operator $H_{\omega/4}$ is invertible on each subspace $D_n$, we can turn this into a difference equation where all coefficients $c_{n,t}$ are determined by the coefficients on the preceding $\omega$ equal-time subspaces, which directly leads to a formulation as an initial-value problem which is uniquely specified by fixing initial conditions on the first $\frac{1}{2}\omega$ equal-time subspaces $D_0$ to $D_{\frac{1}{2}\omega-\frac{1}{2}}$ (although the generic order is $\omega$, for the initial-value problem the order $\frac{1}{2}\omega$ for small $n$ matters; note that $n$ is a half-integer). If $H_{\omega/4}$ is not invertible on some subspace $D_n$, then not all coefficients at time $n$ are specified uniquely by the preceding ones. This can be interpreted as an appearance of a singularity where new boundary conditions have to be given. Note that this can be neither the initial singularity (which would appear at the lowest time values where the initial conditions...
are fixed) nor a turning point where the universe recollapses (at such a point the coefficients at higher times should be given uniquely by the initial-value problem in such a way that they are decreasing sufficiently fast). It could also mean that at this point our internal time ceases to be a good one; the actual interpretation depends on which specific model is considered.

There are a lot of questions which can be asked about the proposed discrete time evolution, most of which can be settled only after studying many models in detail. Maybe the first question coming to mind if one is used to the usual evolution in quantum theory with a fixed background time is whether the evolution is unitary. However, note that this is not possible in the usual way because there is an initial and possibly a final time, which implies that the evolution cannot be described by a unitary operator of the form $\exp(i\hbar^{-1}t \hat{H})$ with a time-independent (for a closed system) Hamiltonian $\hat{H}$ and which would be defined for all times $-\infty < t < \infty$. First, one would have to adapt this to a discrete time in the form of an evolution $U^n$, but this would also imply that each state could be evolved back to negative $n$ by applying $U^{-1}$ arbitrarily often. An initial time together with a unitary evolution can appear only in the sense (e.g. in a first-order formulation, see below) that there is, for any two times $n_1$ and $n_2$, a unitary operator $E_{n_1,n_2}$ which describes the evolution from time $n_1$ to time $n_2$. In order not to be of the form $U^{n_2-n_1}$ and to allow an initial time, the evolution operators have to be time dependent (although the universe as a whole is a closed system), i.e. dependent on $n_1$ and $n_2$, not only on the difference. This is indeed the case for our discrete equations because the decomposition of the holonomy multiplication (e.g. the factor $2^n/(2^n + 1)$ in equation (7)) and the action of the volume operator provide such a dependence on $n$. Note that, whereas in the usual quantum theory time remains forever and does not participate in dynamics, in a quantized generally covariant system time is one of the dynamical degrees of freedom and can be created as well as annihilated. Therefore, even a closed system, which a universe is by definition, must have a time-dependent evolution in this framework.

If we have a unitary evolution in the above sense we can define a physical inner product in the following way: let $s^{(1)}$ and $s^{(2)}$ be two solutions of the Wheeler–DeWitt equation. In general, i.e. if zero lies in the continuous part of the spectrum of the Wheeler–DeWitt operator, their inner product in the kinematical Hilbert space is not defined and both are not square summable in the $\ell^2$-norm. We can, however, define an inner product on the solution space of the constraint by

$$
(s^{(1)}, s^{(2)})_{\text{phys}} := \sum_{i=0}^{\omega-1} \sum_L s^{(1)}_{n_0-i/2,L} s^{(2)}_{n_0-i/2,L}
$$

for a fixed time $n_0 \geq \frac{1}{\sqrt{\omega}}$. If the evolution is unitary the inner product does not depend on the value $n_0$ and defines the physical Hilbert space $\mathcal{H}_{\text{phys}}$. Recalling that the evolution is generated by a constraint and, therefore, related to a gauge transformation, this inner product has the natural interpretation as fixing the gauge by choosing a time $n_0$ and using the kinematical inner product to derive the physical one. In other words, the infinite volume of the ‘gauge’ group has been divided out. In this interpretation, we can also present the physical inner product in terms of a rigging map:

$$
\eta(c^{(1)})[c^{(2)}] := \sum_{i=0}^{\omega-1} \sum_L c^{(1)}_{n_0-i/2,L} c^{(2)}_{n_0-i/2,L}.
$$

Another problem is whether the constraint operator has to be self-adjoint. According to standard quantization procedures, this should be so because it corresponds to a real function on phase space. Nevertheless, in quantum gravity this issue concerning the Hamiltonian constraint
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[19] is still debated. We can give here at least a symmetric ordering of our Wheeler–DeWitt operators in the form

$$\frac{1}{2}((\hat{H} + \hat{H}^*)c)_n = \frac{1}{2} \sum_{i=-\omega/2}^{\omega/2} ((H_i + S_{-i/2}H_i^{(s)}S_{-i/2})c)_{n+i/2}$$

where $^{(s)}$ denotes the adjoint in each equal-time subspace $D_n$ separately (which is the same as * for an operator fixing all of these subspaces), and we used the shift operators $S_j$ with $S_j^* = S_{-j}$ defined by $(S_jc)_n := c_{n+j}$ for $j \geq 0$ and $(S_jc)_n := c_{n+j}$ if $n \geq -j$. $(S_jc)_n := 0$ if $n < j$ for $j < 0$. The issue of self-adjoint extensions can, however, be discussed only in more explicit realizations.

For technical reasons it is interesting to find a first-order formulation of the evolution for which $\omega = 1$. Already for Bianchi models, the order $\omega$ of the dynamical difference equation is rather high (for Bianchi I and IX, for example, there are maximally two factors of holonomies $h_n$ in the Euclidean constraint leading to maximally five factors of $h_n$ in the Lorentzian constraint and thus to an order $\omega = 10$) which is even increased if we go to isotropic models. Note that due to the role of point holonomies in the regularization of the constraint (and due to our selection of an internal time) the order of the difference equation increases if one introduces some degree of isotropy: now rotated holonomies can also contribute to the time spin. Thus, isotropic models have a product of maximally five (flat model) or six (closed model) in the Euclidean constraint, and 13 or 15 in the Lorentzian constraint leading to an evolution equation of the order of 26 or 30. There are two possibilities to reduce the order (at least formally): in special cases one could try to take a root, i.e. write the equation in the form $$(\Delta c)_n := (\Delta c)_n = 0$$

where

$$(\Delta c)_n := c_{n+\frac{1}{2}H^\omega} - c_n$$

is the difference operator and $H$ can be interpreted as a Hamiltonian. The second possibility, which always works, is to formulate a matrix difference equation for the column vectors

$$v_n := \begin{pmatrix} c_{n+\frac{1}{2}} \\ \vdots \\ c_n \end{pmatrix}$$

which have less non-vanishing components for small $n$, spanning the equal-time subspace $D_n$. In both cases a general solution of the first-order difference equation leads to evolution operators

$$E_{n_1,n_2}: D_{n_1} \rightarrow D_{n_2}$$

which describe the evolution from time $n_1$ to time $n_2$.

Assuming such a first-order formulation we will now discuss the issue of physical observables.

4. Evolving observables

When there is a dynamical formulation of some model system, one is interested in the evolution and possible values (in quantum theory spectra and expectation values) of observables. Most interesting in the present context is the volume, because we would like to know whether the discrete kinematical spectrum is also significant in the physical Hilbert space where states solve the Wheeler–DeWitt equation. In the discussion of homogeneous quantum geometry [15] we
ignored the Hamiltonian constraint, but now in a quantum gravitational model all observables have to commute with this constraint, which is not the case for the kinematical volume operator. One can see this by determining the eigenstates of the volume operator which, in the dreibein representation, is given by $(\hat{V} e)_{n,L} = V(n, L)c_{n,L}$ (provided the spin network basis by means of which the transition to the dreibein representation has been performed has been chosen as containing only volume eigenstates, which is always possible) where the real function $V(n, L)$ is not known explicitly for the Bianchi models but depends only on the labels $(n, L)$. We can thus immediately read off the eigenstates $c_{n,L}^{(n_0, L_0)} = \delta_{n_0,n}\delta_{L_0,L}$ to the eigenvalues $V(n_0, L_0)$ (possibly degenerate). This shows that the (kinematical) volume eigenstates have vanishing coefficients on all but a fixed equal-time subspace $D_n$ and cannot be solutions of the discrete evolution equation.

Within the framework of classical minisuperspaces (or other generally covariant systems) and their standard quantizations there, several definitions have been proposed of what has to be understood as physical observables subject to a relational evolution with respect to another observable [10, 20]. We use and recall here the method given in [10] because it has been applied there to the Bianchi I model such that we will be able to compare this construction in a standard minisuperspace quantization with an analogous one in a discrete time context. Given a classical function $\hat{O}$ on the kinematical phase space of the model (so that it is not necessarily a physical observable) which does not depend on the canonical conjugate of the selected internal time (in an external time formalism such a dependence would be impossible, anyway, but here we have to impose this condition because time and also its conjugate are chosen from, or functions of, the usual phase space coordinates), one first has to quantize it to an operator $\hat{\hat{O}}$ acting on wavefunctions schematically written as $\psi(a, \phi)$. As earlier, $a$ denotes the internal time and $\phi$ the remaining degrees of freedom. Because $\hat{\hat{O}}$ is not assumed to be an observable, $\hat{\hat{\psi}}$ is in general not a physical state even if $\hat{\psi}$ is so. For simplicity, we now make the following assumptions about the evolution: $a = e^t$ is the (positive) scale factor and the evolution is given in a first-order formulation by the Schrödinger-like equation $i\hbar \frac{\partial \hat{\psi}}{\partial t} = \hat{H} \hat{\psi}$ with a self-adjoint Hamiltonian $\hat{H}$. Note that the evolution equation is written in the time parameter $t = \log a$ which is unbounded from above and below such that there are no obstructions to a unitary evolution with respect to this parameter.

From the operator $\hat{\hat{O}}$ one can construct an ‘evolving observable’ $\hat{\hat{O}}(t)$, a family of operators depending on the parameter $t$ [10]. However, this should not be confused with the operator $\hat{\hat{O}}$ in the Heisenberg picture (which just would be an equivalent description of the same operator); for now both the operator representing an evolving observable and the wavefunction depend on the internal time: the wavefunction describes the entire history of the system which is changed for now both the operator representing an evolving observable in the Heisenberg picture (which just would be an equivalent description of the same operator); depending on the parameter $t$

$$\delta_{n_0,n}\delta_{L_0,L}$$

the time parameter $t$

To construct the evolving observable $\hat{\hat{O}}(t)$ suppose that a solution $\hat{\psi}$ of the Wheeler–DeWitt equation is given. For $\hat{\hat{O}}(t_0)$ to be a physical observable it has to map the physical state $\hat{\psi}$ to another physical state $\hat{\hat{O}}(t_0)\hat{\psi}(a, \phi)$ which will be achieved in the following way: first fix the internal time $t = t_0$ and apply the given operator $\hat{\hat{O}}$ to the ‘equal-time wavefunction’ $\hat{\psi}(a = e^{t_0}, \phi)$ (this is possible because $\hat{\hat{O}}$, assumed not to depend on the conjugate of time, does not contain derivatives $\frac{\partial}{\partial a}$) and evolve the resulting function to arbitrary times $t$, i.e.

$$[\hat{\hat{O}}(t_0)\hat{\psi}](a = e^t, \phi) := \exp \left( -i\hbar^{-1}(t - t_0)\hat{H} \right) \hat{\psi}(a = e^{t_0}, \phi).$$

By construction, the right-hand side is a physical state and so $\hat{\hat{O}}(t)$ is an observable. Note that kinematical expectation values of the operator $\hat{\hat{O}}$ are directly related to the physical expectation values of $\hat{\hat{O}}(t)$ only if $\hat{\hat{O}}$ commutes with the Hamiltonian $\hat{H}$ where, of course, eigenvalues of the evolving observable are functions of the internal time describing a relational evolution of some degree of freedom with respect to $a$. An example for such an observable in the above
model is the volume which is just given by multiplication with $e^t$; as a parameter-dependent multiple of the identity operator it is, however, not quite interesting because it describes the ‘evolution of the volume with respect to the volume’. Nevertheless, it shows that for the scale factor all positive real values are allowed, i.e. there is no discrete volume spectrum.

We are now going to present a similar construction for loop quantum cosmology where we are, in particular, interested in the implications of discrete time. Our starting point is similar to the one above: we have a kinematical operator $\hat{O}$ and a solution $s$ of the Wheeler–DeWitt equation given in the dreibein representation by the coefficients $s_{n,L}$ where $n$ is the discrete time label. Again we assume the evolution to be given in a first-order formulation by the evolution operators $E_{n_1,n_2}: D_{n_1} \rightarrow D_{n_2}$ of equation (12). The same procedure as above is to fix the internal time $n = n_0$, apply the kinematical operator, and evolve to arbitrary time labels:

$$\left(\hat{O}(n) s\right)_{n,L} = \left(E_{n_0,n} \hat{O} s\right)_{|n=n_0}$$

(13)

where $s_{|n=n_0}$ is the restriction of $s$ to the subspace $D_{n_0}$. This construction works for any kinematical operator which preserves every subspace $D_n$, analogous to the condition that $\hat{O}$ must not depend on the conjugate of time (e.g. in Bianchi models this is the case for any operator not containing the holonomy $h_1$ which changes the time label $n = j_i$).

An immediate consequence of the construction together with our discrete time formulation is that only discrete values for the parameter $n$ in evolving observables $\hat{O}(n)$ are allowed, so evolution is always with respect to a discrete time. Most interesting in cosmological models is the volume which is kinematically quantized by the operator $\hat{V}$ and has a discrete spectrum [15]. We can apply the construction of an evolving volume operator $\hat{V}(n)$ which describes the evolution of the volume with respect to discrete time $n$ (because now time is not chosen to be the scale factor, the relational evolution $V(n)$ is non-trivial). Most important, also for the full theory, is the question of whether the spectrum of this evolving volume is again discrete and somehow related to the kinematical spectrum.

In order to make the relation between kinematical and physical spectra more precise, we now introduce some formalism. We write the evolution as an operator $E_{n_0}$ which, acting on a state $d$ in the ‘initial’ subspace $D_{n_0}$, yields a complete history given by a physical state:

$$E_{n_0}: D_{n_0} \rightarrow \mathcal{H}_{\text{phys}}, \quad (E_{n_0} d)_{n,L} = (E_{n_0,n} d)_{|L}.$$  

Because $(E_{n_0} d)_{|n=n_0} = d$ in general and $E_{n_0}, (s_{|n=n_0}) = s$ for a physical state $s$, $E_{n_0}$, is the inverse of the projection operator

$$\pi_{n_0}: \mathcal{H}_{\text{phys}} \rightarrow D_{n_0}, \quad s \mapsto s_{|n=n_0}$$

acting on physical states in $\mathcal{H}_{\text{phys}}$. On the kinematical Hilbert space $\mathcal{H}_{\text{kin}}$, $\pi_{n_0}$ is not invertible but we can easily calculate its adjoint

$$\iota_{n_0}: D_{n_0} \rightarrow \mathcal{H}_{\text{kin}}, \quad (\iota_{n_0} d)_{n,L} := \delta_{n,n_0} d_L$$

which is just the inclusion map of $D_{n_0}$ as a subspace of $\mathcal{H}_{\text{kin}}$. From the equation

$$(\epsilon, \iota_{n_0} d) = \sum_{n,L} \epsilon_{n,L} \delta_{n_0,n} d_L = \sum_{L} \epsilon_{n_0,L} d_L = (\pi_{n_0} \epsilon, d)$$

we directly infer $\pi_{n_0}^* = \iota_{n_0}$ (both operators are bounded).

We can now write an evolving observable constructed from a kinematical operator $\hat{O}$ as

$$\hat{O}(n) = E_{n_0} \circ \hat{O} \circ \pi_{n}.$$  

(14)

Of physical interest are the expectation values $(s, \hat{O}(n)s)_{\text{phys}}$ which, provided $s$ is a physical state, describe the relational evolution of the observable $O$ with respect to discrete time $n$ in
the given history. These expectation values are directly related to the physical spectrum of \( O \).
In contrast, the kinematical spectrum of \( O \) is directly related to the expectation values \( \langle d, \hat{O}d \rangle \)
of the kinematical operator \( \hat{O} \) in an equal-time subspace \( D_n \). Choosing a physical state \( s \) with \( \pi_n s = d \) and using the above definitions and adjointness relations, we can write this as

\[
\langle d, \hat{\pi}_n s \rangle = \langle d, \pi_n E_n, \hat{\pi}_n s \rangle = \langle i d, \hat{O}(n)s \rangle
\]

and see that the kinematical expectation values are given by matrix elements of \( \hat{O}(n) \) with respect to an unphysical state \( \iota d \) and a physical state \( s \). This immediately shows that the kinematical expectation values do not have any physical meaning.

Although individual expectation values in a given physical state are unrelated to kinematical ones and a computation of an evolving expectation value \( \langle s, \hat{O}(n)s \rangle \) in a given history \( s \) can be very complicated, it is simpler to study the set of possible outcomes of expectation values, i.e. the spectrum, of an observable \( \hat{O}(n) \) at a fixed parameter \( n \). To that end, we proceed in the following way, using the example of the volume operator: we fix an \( n_0 \) and diagonalize the kinematical volume operator \( \hat{V} \) on the equal-time subspace \( D_{n_0} \).

Because we need a first-order formulation in order to define \( \hat{V}(n_0) \), we assume \( D_{n_0} \) to be the space of \( \omega \)-column vectors \( v_{n_0} \) of equation (11). Eigenstates of \( \hat{V} \) in \( D_{n_0} \) are denoted as \( v^{(i)} \), \( 0 \leq i \leq \omega - 1 \), and fulfill the eigenvalue equation \( \hat{V}v^{(i)} = V(n_0 - \frac{1}{2}i, L)v^{(i)} \) with the kinematical eigenvalues \( V(n, L) \).

We can then evolve each of these eigenvectors to complete histories \( s^{(n_0,i,L)}(n_0,i,L) \) which form a complete set in the physical Hilbert space. By definition, we have

\[
\hat{V}(n_0)s^{(n_0,i,L)} = E_{n_0, V}V(n_0 - \frac{1}{2}i, L)v^{(i,L)} = V(n_0 - \frac{1}{2}i, L)s^{(n_0,i,L)}
\]

(15)
demonstrating that the kinematical eigenvalues are also the physical ones. Of course, this does not tell us anything about evolution because this is coded in the dependence on \( n \) of expectation values of \( \hat{V}(n) \) in a fixed physical state (the set of eigenstates used above is \( n \)-dependent). However, it shows that kinematical spectra are relevant for physical operators. We have here the first models where a discrete spectrum of a metrical operator in the physical Hilbert space has been derived. Note, however, that our conclusion depends on the assumption that the spin \( n = j_1 \), or another combination of the spin labels, defines a sensible time variable.

5. Discussion

Although we did not discuss any particular model but concentrated on conceptual issues, it has by now become clear that our proposal of loop quantum cosmology is very different from the standard minisuperspace quantum cosmology. In view of the discrete structure of space revealed in loop quantum gravity this is what one would intuitively expect because then also time should be discrete, implying departures from the conventional continuous time of quantum mechanics. We emphasize here that, whereas the standard quantizations are equivalent to the treatment of (relativistic) quantum mechanical systems and rely heavily on methods which are assumed to be inapplicable in a full quantization of general relativity, our attitude was always to be as close to the general framework of the loop quantization of general relativity as possible. In this sense, we regard results of loop quantum cosmology as being more trustworthy for an extrapolation of minisuperspace results to the full theory. Manifestations of the close relationship to full loop quantum gravity are the discrete geometric spectra and the very similar Hamiltonian constraint operators. This lead us to the derivation of a discrete time evolution and of discrete physical spectra of geometric operators as new contributions to the loop quantization programme.
In contrast to standard minisuperspace quantizations we did not perform the symmetry reduction directly at the classical level, but were able to interpret the states as symmetric states in the kinematical sector of a quantization of the full theory leading to a preservation of discrete geometric spectra. However, still, the symmetry reduction is very restrictive which can be observed in the phenomenon of level splitting, whereas the full volume spectrum is almost continuous for large eigenvalues (they are given by arbitrary sums of irrational numbers, the distance between subsequent ones can be made arbitrarily small at sufficiently high values), the reduction to homogeneity leads to a degeneration probably undoing the almost continuity (the spectrum is not known explicitly, however); for the highest symmetry, isotropy, the distance between subsequent levels even increases with increasing eigenvalues [15]. Nevertheless, the relative difference decreases as \( j^{-3/2} [(j + 1)^{3/2} - j^{3/2}] \sim \frac{k}{2} j^{-1} \), which still can be sufficient to recover the usual classical continuous space for large volumes (compare with energy levels of the harmonic oscillator). Anyway, quantum cosmological models are most interesting for small volumes, i.e. close to the classical singularity, where the discreteness of both the full and the symmetric spectra can be expected to be relevant.

5.1. Comparison with the full theory

Of course, as compared with the full theory we are in a very special situation if we are studying the dynamics of homogeneous models because, first and foremost, we have a natural candidate for an explicit internal time. This fact enabled our discussion of the dynamics of loop quantum cosmology. Another simplification comes from the reduction of degrees of freedom leading to models which are defined on a fixed simple graph. Future analytical and numerical computations will benefit from this reduction.

On the other hand, Wheeler–DeWitt operators of homogeneous models [5] are very similar to a single-vertex contribution of the operator in the full theory [2]. Therefore, their analysis will not be much simpler. However, even without having explicit solutions of the Wheeler–DeWitt equation we were able to derive consequences for the evolution, which hopefully will help to shed light on the dynamics of the full theory.

5.2. Difference versus differential evolution equations

The main discrepancy between standard minisuperspace quantizations and the one presented here is that time evolution is described by a differential equation for the former and by a difference equation for the latter ones. For a numerical analysis this makes no difference because differential equations, if they cannot be solved analytically, are discretized anyway.

Conceptually, the following question may be more interesting, namely whether our discrete time evolution equations can be interpreted as a discretization of a continuous (semiclassical) time evolution. If this is possible, the continuous-time formulation would be of relevance for a discussion of the classical limit. However, this problem is highly non-unique which implies that there may be different continuum pictures described by one and the same discrete evolution equation.

Such a behaviour is also suggested by the problem of consistency which often has to be faced in numerics (see, e.g., [21]). If a differential equation is discretized for a numerical analysis, it is possible that a solution converges to a solution of another differential equation if the discretization is refined. In particular, for higher-order approximation schemes, there are additional and often very weird solutions which have to be under control in a sensible code.

Recall that our discrete equations (9) are usually of a very high-order compared with the order two of the differential Wheeler–DeWitt equations. Although by itself this is no
obstruction to recovering a standard low-order differential equation, it implies that we have to expect in general very many solutions which can have no classical counterparts. Note that, contrary to the numerical analysis of a differential equation where additional solutions of its discretization have to be suppressed, in our context the discrete description is regarded as being more fundamental. Therefore, additional solutions have to be suppressed only in semiclassical regimes; they are genuinely quantum ones and may be of relevance for a discussion of quantum modifications of the classical singularity.

5.3. Avoiding the classical singularity

The high order of our discrete equations has a consequence for the question of whether there is always a positive probability for a physical history to have a singularity. Under ‘singularity’ we will in this context understand a geometry with vanishing volume, i.e. we ask whether there is for each physical state \( s \) an \( n_0 \) such that \( \hat{V}(n_0)s = 0 \). Because the evolution is linear, this is the case if the kinematical volume operator \( \hat{V} \) applied to an equal-time slice of the physical state \( s \) is zero: \( \hat{V}\pi_{n_0}s = 0 \) with \( \pi_{n_0}s \neq 0 \).

On the classical side, there are the singularity theorems [22] which state that any classical spacetime has a singularity under some conditions on the matter content (and the cosmological constant). In Bianchi models a singularity is generic, whereas isotropic models have a singularity only if matter is coupled which fulfils a certain positive-energy condition (which may also have to compensate a positive cosmological constant). Without matter, spatially isotropic spacetimes are maximally symmetric (Minkowski, de Sitter or anti-de Sitter space) and thus cannot have a singularity (except for coordinate singularities which are introduced by an inappropriate slicing or time coordinate). The question is now whether there is a quantum analogue of these theorems or whether a singularity can be avoided there in the sense that the probability for a universe to be in a singular geometry vanishes.

In Bianchi models, the kernel of the volume operator is very large, even for positive times \( n > 0 \) such that a discussion here is impossible without explicit solutions of the Wheeler–DeWitt equation in a specific model.

In isotropic models, however, there are only three states with zero volume [15]. The order of the discrete evolution equation, on the other hand, is much higher so that we can easily demand that the amplitude \( s_{n,L} \), where \( L \) denotes the insertion and matter labels, of a physical state vanishes in these degenerate states thus avoiding the singularity. Note that this is independent of the matter coupled to the isotropic model as long as time is made only of gravitational degrees of freedom as we did above. Thus we see, that also for matter which classically inevitably leads to a singularity a degenerate geometry can always be avoided in quantum solutions of isotropic models. However, as already discussed, the high-order discrete equations governing the quantum time evolution have a wealth of solutions, most of which will not correspond to classical ones. Therefore, also in isotropic models an avoidance of the singularity can be concluded only if one finds a solution which has vanishing amplitudes on the degenerate geometries and corresponds to a classical solution for large volumes.

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