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Loop Quantum Cosmology

Martin Bojowald
Institute for Gravitation and the Cosmos
The Pennsylvania State University
University Park, PA 16802, U.S.A.
and
Max Planck Institute for Gravitational Physics
(Albert Einstein Institute)
Am Mühlenberg 1, 14476 Potsdam, Germany
email: bojowald@gravity.psu.edu

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Abstract

Quantum gravity is expected to be necessary in order to understand situations in which classical general relativity breaks down. In particular in cosmology one has to deal with initial singularities, i.e., the fact that the backward evolution of a classical spacetime inevitably comes to an end after a finite amount of proper time. This presents a breakdown of the classical picture and requires an extended theory for a meaningful description. Since small length scales and high curvatures are involved, quantum effects must play a role. Not only the singularity itself but also the surrounding spacetime is then modified. One particular theory is loop quantum cosmology, an application of loop quantum gravity to homogeneous systems, which removes classical singularities. Its implications can be studied at different levels. The main effects are introduced into effective classical equations, which allow one to avoid the interpretational problems of quantum theory. They give rise to new kinds of early-universe phenomenology with applications to inflation and cyclic models. To resolve classical singularities and to understand the structure of geometry around them, the quantum description is necessary. Classical evolution is then replaced by a difference equation for a wave function, which allows an extension of quantum spacetime beyond classical singularities. One main question is how these homogeneous scenarios are related to full loop quantum gravity, which can be dealt with at the level of distributional symmetric states. Finally, the new structure of spacetime arising in loop quantum gravity and its application to cosmology sheds light on more general issues, such as the nature of time.

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Contents

1 Introduction

Die Grenzen meiner Sprache bedeuten die Grenzen meiner Welt.

(*The limits of my language mean the limits of my world.*)

Ludwig Wittgenstein
Tractatus logico-philosophicus

While general relativity is very successful in describing gravitational interaction and the structure of space and time on large scales [308], quantum gravity is needed for small-scale behavior. This is usually relevant when curvature, or in physical terms energy densities and tidal forces, becomes large. In cosmology this is the case close to the Big Bang as well as in the interior of black holes. We are thus able to learn about gravity on small scales by looking at the early history of the universe.

Starting with general relativity on large scales and evolving backward in time, the universe becomes smaller and smaller and quantum effects eventually dominate. Singularity theorems illustrate that classical gravitational theory by itself cannot be sufficient to describe the development of the universe in a well-defined way [178]. After a finite time of backward evolution, the classical universe will collapse into a single point and energy densities will diverge. At this point, classic gravitational theory breaks down and cannot be used to determine what is happening. Quantum gravity, with its different dynamics on small scales, is expected to solve this problem.

The quantum description presents not only a modified dynamical behavior on small scales, but also a new conceptual setting. Rather than dealing with a classical spacetime manifold, we now have evolution equations for the wave function of a universe. This opens up a vast number of problems on various levels from mathematical physics to cosmological observations, and even philosophy. This review is intended to give an overview and summary of the current status of those problems, in particular in the new framework of loop quantum cosmology.

2 The Viewpoint of Loop Quantum Cosmology

Loop quantum cosmology is based on quantum Riemannian geometry, or loop quantum gravity [254, 23, 293, 256], which is an attempt at a non-perturbative and background-independent quantization of general relativity. This means that no assumption of small fields or the presence of a classical background metric are made, both of which are expected to be essential close to classical singularities at which the gravitational field diverges and space degenerates. In contrast to other approaches to quantum cosmology, there is a direct link between cosmological models and the full theory [46, 96], as we will describe later in Section 7. With cosmological applications we are thus able to test several possible constructions and draw conclusions for open issues in the full theory. At the same time, of course, we can learn about physical effects, which have to be expected from properties of the quantization and can potentially lead to observable predictions. Since the full theory is not completed yet, however, an important issue in this context is the robustness of those applications to choices in the full theory and quantization ambiguities.

The full theory itself is, understandably, extremely complex and thus requires approximation schemes for direct applications. Loop quantum cosmology is based on symmetry reduction, in the simplest case to isotropic geometries [54]. This poses the mathematical problem of how the quantum representation of a model and its composite operators can be derived from that of the full theory, and in which sense this can be regarded as an approximation with suitable correction terms. Research in this direction currently proceeds by studying symmetric models with fewer symmetries and the relationships between them. This allows one to see what role anisotropies and inhomogeneities play in the full theory.

While this work is still in progress, one can obtain full quantizations of models by using basic features, as they can already be derived from the full theory together with constructions of more complicated operators in a way analogous to what one does in the full theory (see Section 5). For these complicated operators, the prime example being the Hamiltonian constraint, which dictates the dynamics of the theory, the link between a model and the full theory is not always clear-cut. Nevertheless, one can try different versions of specific Hamiltonian constraints in the model in explicit ways and see what implications this has; the robustness issue arises again. This has already been applied to issues such as the semiclassical limit and general properties of quantum dynamics as described in Section 6. Thus, general ideas, which are required for this new, background-independent quantization scheme, can be tried in a rather simple context, in explicit ways, in order to see how those constructions work in practice.

At the same time, there are possible phenomenological consequences to the physical systems being studied, which are the subject of Section 4. In fact, it turned out, rather surprisingly, that already very basic effects, such as the discreteness of quantum geometry (and other features briefly reviewed in Section 3, for which a reliable derivation from the full theory is available), have very specific implications for early-universe cosmology. While quantitative aspects depend on quantization ambiguities, there is a rich source of qualitative effects, which work together in a well-defined and viable picture of the early universe. In this way, as later illustrated, a partial view of the full theory and its properties emerges from a physical as well as a mathematical perspective.

With this wide range of problems being investigated, we must keep our eyes open to input from all sides. There are mathematical-consistency conditions in the full theory, some of which are identically satisfied in the simplest models (such as the isotropic model, which has only one Hamiltonian constraint and thus a trivial constraint algebra). They are being studied in different, more complicated models and also in the full theory directly. Since the conditions are not easy to satisfy, they put stringent bounds on possible ambiguities. From physical applications, on the other hand, we obtain conceptual and phenomenological constraints, which can be complementary to those obtained from consistency checks. All this contributes to a test and better understanding of the background-independent framework and its implications.

Other reviews of loop quantum cosmology at different levels can be found in [64, 63, 297, 58, 99, 59, 141, 67, 145, 15, 110]. For complementary applications of loop quantum gravity to cosmology see [204, 205, 2, 167, 222, 1].

3 Loop Quantum Gravity

Since many reviews of full loop quantum gravity [254, 293, 23, 256, 242], as well as shorter accounts [9, 10, 255, 284, 248, 296], are already available, we describe here only those properties that will later on be essential. Nevertheless, this review is mostly self-contained; our notation is closest to that in [23]. A recent bibliography can be found in [137].

3.1 Geometry

General relativity in its canonical formulation [6] describes the geometry of spacetime in terms of fields on spatial slices. Geometry on such a spatial slice Σ is encoded in the spatial metric q_{ab}, which presents the configuration variables. Canonical momenta are given in terms of the extrinsic curvature K_{ab}, which is the derivative of the spatial metric with respect to changes in the spatial slice. These fields are not arbitrary, since they are obtained from a solution of Einstein's equations by choosing a time coordinate defining the spatial slices, and spacetime geometry is generally covariant. In the canonical formalism this is expressed by the presence of constraints on the fields: the diffeomorphism constraint and the Hamiltonian constraint. The diffeomorphism constraint generates deformations of a spatial slice or coordinate changes, and, when it is satisfied, spatial geometry does not depend on the space coordinates chosen. General covariance of spacetime geometry for the time coordinate is then completed by imposing the Hamiltonian constraint. Furthermore, this constraint is important for the dynamics of the theory; since there is no absolute time, there is no Hamiltonian generating evolution, but only the Hamiltonian constraint. When it is satisfied, it encodes correlations between the physical fields of gravity and matter, such that evolution in this framework is relational. The reproduction of a spacetime metric in a coordinate-dependent way then requires one to choose a gauge and to compute the transformation in gauge parameters (including the coordinates) generated by the constraints.

It is often useful to describe spatial geometry not by the spatial metric but by a triad e_i^a, which defines three vector fields orthogonal to each other and normalized at each point. This specifies all information about the spatial geometry, and indeed the inverse metric is obtained from the triad by $q^{ab} = e_i^a e_i^b$, where we sum over the index i, counting the triad vector fields. There are differences, however, between metric and triad formulations. First, the set of triad vectors can be rotated without changing the metric, which implies an additional gauge freedom with group SO(3) acting on the index i. Invariance of the theory under rotations is then guaranteed by a Gauss constraint in addition to the diffeomorphism and Hamiltonian constraints.

The second difference will turn out to be more important later on. Not only can we rotate the triad vectors, we can also reflect them, i.e., change the orientation of the triad given by $\mathrm{sign}\,(\det\,(e_i^a))$. This does not change the metric either and so could be included in the gauge group as O(3). However, reflections are not connected to the unit element of O(3) and thus are not generated by a constraint. It then has to be seen whether or not the theory allows one to impose invariance under reflections, i.e., if its solutions are reflection symmetric. This is not usually an issue in the classical theory since positive and negative orientations on the space of triads are separated by degenerate configurations in which the determinant of the metric vanishes. Points on the boundary are usually singularities at which the classical evolution breaks down such that both sides will never connect. However, since one expects that quantum gravity may resolve classical singularities, which is indeed confirmed in loop quantum cosmology, we will have to keep this issue in mind and not restrict ourselves to only one orientation from the outset.

3.2 Ashtekar variables

To quantize a constrained canonical theory one can use Dirac's prescription [153] and first represent the classical Poisson algebra of a suitable complete set of basic variables on phase space as an operator algebra on a Hilbert space, called kinematical. This ignores the constraints, which can be written as operators on the same Hilbert space. At the quantum level, the constraints are then solved by determining their kernel, and the solution space has to be equipped with an inner product to provide the physical Hilbert space. If zero is in the discrete part of the spectrum of a constraint, as in the Gauss constraint when the structure group is compact, the kernel is a subspace of the kinematical Hilbert space to which the kinematical inner product can be restricted. If, on the other hand, zero lies in the continuous part of the spectrum, there are no normalizable eigenstates and one has to construct a new physical Hilbert space from distributions. This is the case for the diffeomorphism and Hamiltonian constraints. The main condition for the physical inner product is that it allows one to quantize real-valued observables. To perform the first step, we need a Hilbert space of functionals $\psi[q]$ of spatial metrics, as is proposed in Wheeler–DeWitt quantizations; see, e.g., [310, 173]. Unfortunately, the space of metrics, or, alternatively, extrinsic curvature tensors, is poorly understood mathematically and not much is known about suitable inner products. At this point, a new set of variables introduced by Ashtekar [7, 8, 37] becomes essential. This is a triad formulation, but uses the triad in a densitized form, i.e., it is multiplied by an additional factor of a Jacobian under coordinate transformations. The densitized triad E^a_i is then related to the triad by $E^a_i = \left|\det e^b_j\right|^{-1} e^a_i$ but has the same properties concerning gauge rotations and its orientation (note the absolute value, which is often omitted). The densitized triad is canonically conjugate to extrinsic curvature coefficients $K^i_a := K_{ab}e^b_i$:

$$\{K^i_a(x), E^b_j(y)\} = 8\pi G\delta^b_a\delta^i_j\delta(x,y) \tag{1}$$

where G is the gravitational constant. The extrinsic curvature is then replaced by the Ashtekar connection

$$A^i_a = \Gamma^i_a + \gamma K^i_a \tag{2}$$

with a positive value for γ, the Barbero–Immirzi parameter [37, 193]. Classically, this number can be changed by a canonical transformation of the fields, but it will play a more important and fundamental role upon quantization. The Ashtekar connection is defined in such a way that it is conjugate to the triad,

$$\{A^i_a(x), E^b_j(y)\} = 8\pi\gamma G\delta^b_a\delta^i_j\delta(x,y) \tag{3}$$

and obtains its transformation properties as a connection from the spin connection

$$\Gamma^i_a = -\epsilon^{ijk}e^b_j(\partial_{[a}e^k_{e]} + \tfrac{1}{2}e^c_k e^l_a\partial_{[c}e^l_{b]})\,. \tag{4}$$

(In a first-order formulation there are additional contributions from torsion in the presence of fermionic matter; see, e.g., [76] for details.)

Spatial geometry is then obtained directly from the densitized triad, which is related to the spatial metric by

$$E^a_i E^b_i = q^{ab}\det q\,.$$

There is more freedom in a triad since it can be rotated without changing the metric. The theory is independent of such rotations, provided the Gauss constraint,

$$G[\Lambda] = \frac{1}{8\pi\gamma G}\int_\Sigma \mathrm{d}^3x\,\Lambda^i D_a E^a_i = \frac{1}{8\pi\gamma G}\int_\Sigma \mathrm{d}^3x\,\Lambda^i(\partial_a E^a_i + \epsilon_{ijk}A^j_a E^a_k) \approx 0, \tag{5}$$

is satisfied. Independence from any spatial coordinate system or background is implemented by the diffeomorphism constraint (modulo Gauss constraint)

$$D[N^a] = \frac{1}{8\pi\gamma G}\int_\Sigma \mathrm{d}^3x N^a F^i_{ab}E^b_i \approx 0 \tag{6}$$

with the curvature F^i_{ab} of the Ashtekar connection. In this setting, one can then discuss spatial geometry and its quantization.

Spacetime geometry, however, is more difficult to deduce, since it requires a good knowledge of the dynamics. In a canonical setting, the dynamics are implemented by the Hamiltonian constraint

$$H[N] = \frac{1}{16\pi\gamma G}\int_\Sigma \mathrm{d}^3x\, N\, |\det E|^{-1/2}\left(\epsilon_{ijk}F^i_{ab}E^a_jE^b_k - 2(1+\gamma^2)K^i_{[a}K^j_{b]}E^a_iE^b_j\right) \approx 0, \tag{7}$$

where extrinsic-curvature components have to be understood as functions of the Ashtekar connection and the densitized triad through the spin connection.

3.3 Representation

The key new aspect now is that we can choose the space of Ashtekar connections as our configuration space, whose structure is much better understood than that of a space of metrics. Moreover, the formulation lends itself easily to background-independent quantization. To see this we need to remember that quantizing field theories requires one to smear fields, i.e., to integrate them over regions in order to obtain a well-defined algebra without δ-functions, as in Equation (3). This is usually done by integrating both configuration and momentum variables over three-dimensional regions, which requires an integration measure. This is no problem in ordinary field theories, which are formulated on a background such as Minkowski or a curved space. However, doing this here for gravity in terms of Ashtekar variables would immediately spoil any possible background independence since a background would already occur at this very basic step.

There is now a different smearing available that does not require a background metric. Instead of using three-dimensional regions we integrate the connection along one-dimensional curves e and exponentiate in a path-ordered manner, resulting in holonomies

$$h_e(A) = \mathcal{P}\exp\int_e \tau_i A^i_a \dot{e}^a\,\mathrm{d}t \tag{8}$$

with tangent vector $\dot{e}^a$ to the curve e and $\tau_j = -\frac{1}{2}i\sigma_j$ in terms of Pauli matrices. The path-ordered exponentiation needs to be done in order to obtain a covariant object from the non-Abelian connection. The prevalence of holonomies or, in their most simple gauge-invariant form as Wilson loops $\mathrm{tr}h_e(A)$ for closed e, is the origin of loop quantum gravity and its name [258]. Similarly, densitized vector fields can naturally be integrated over two-dimensional surfaces, resulting in fluxes

$$F_S(E) = \int_S \tau^i E^a_i n_a\,\mathrm{d}^2y \tag{9}$$

with the co-normal n_a to the surface.

The Poisson algebra of holonomies and fluxes is now well defined and one can look for representations on a Hilbert space. We also require diffeomorphism invariance, i.e., there must be a unitary action of the diffeomorphism group on the representation by moving edges and surfaces in space. This is required since the diffeomorphism constraint has to be imposed later. Under this condition, together with the assumption of cyclicity of the representation, there is even a unique representation that defines the kinematical Hilbert space [263, 264, 245, 265, 266, 166, 213]. (See [301], however, for examples of other, non-cyclic representations.)

We can construct the Hilbert space in the representation where states are functionals of connections. This can easily be done by using holonomies as "creation operators" starting with a "ground state", which does not depend on connections at all. Multiplying with holonomies then generates states that do depend on connections but only along the edges used in the process. These edges can be collected in a graph appearing as a label of the state. An independent set of states is given by spin-network states [261] associated with graphs, whose edges are labeled by irreducible representations of the gauge group SU(2), in which to evaluate the edge holonomies, and whose vertices are labeled by matrices specifying how holonomies leaving or entering the vertex are multiplied together. The inner product on this state space is such that these states, with an appropriate definition of independent contraction matrices in vertices, are orthonormal.

Spatial geometry can be obtained from fluxes representing the densitized triad. Since these are now momenta, they are represented by derivative operators with respect to values of connections on the flux surface. States, as constructed above, depend on the connection only along edges of graphs, such that the flux operator is non-zero only if there are intersection points between its surface and the graph in the state it acts on [212]. Moreover, the contribution from each intersection point can be seen to be analogous to an angular momentum operator in quantum mechanics, which has a discrete spectrum [21]. Thus, when acting on a given state, we obtain a finite sum of discrete contributions and thus a discrete spectrum of flux operators. The spectrum depends on the value of the Barbero–Immirzi parameter, which can accordingly be fixed using implications of the spectrum such as black-hole entropy, which gives a value on the order of, but smaller than, one [11, 12, 158, 225]. Moreover, since angular-momentum operators do not commute, flux operators do not commute in general [18]. There is, thus, no triad representation, which is another reason that using a metric formulation and trying to build its quantization with functionals on a metric space is difficult.

There are important basic properties of this representation, which we will use later on. First, as already noted, flux operators have discrete spectra and, secondly, holonomies of connections are well-defined operators. It is, however, not possible to obtain operators for connection components or their integrations directly but only in the exponentiated form. These are the direct consequence of background-independent quantization and translate to particular properties of more complicated operators.

3.4 Function spaces

A connection 1-form A_a^i can be reconstructed uniquely if all its holonomies are known [172]. It is thus sufficient to parameterize the configuration space by matrix elements of h_e for all edges in space. This defines an algebra of functions on the infinite-dimensional space of connections $\mathcal{A}$, which are multiplied as $\mathbb{C}$-valued functions. Moreover, there is a duality operation by complex conjugation, and if the structure group G is compact a supremum norm exists, since matrix elements of holonomies are then bounded. Thus, matrix elements form an Abelian C^*-algebra with unit as a sub-algebra of all continuous functions on $\mathcal{A}$.

Any Abelian C^*-algebra with unit can be represented as the algebra of *all* continuous functions on a compact space $\bar{\mathcal{A}}$. The intuitive idea is that the original space $\mathcal{A}$, which has many more continuous functions, is enlarged by adding new points to it. This increases the number of continuity conditions and thus shrinks the set of continuous functions. This is done until only matrix elements of holonomies survive when continuity is imposed, and it follows from general results that the enlarged space must be compact for an Abelian unital C^*-algebra. We thus obtain a compactification $\bar{\mathcal{A}}$, the space of generalized connections [24], which densely contains the space $\mathcal{A}$.

There is a natural diffeomorphism invariant measure $\mathrm{d}\mu_{\mathrm{AL}}$ on $\bar{\mathcal{A}}$, the Ashtekar–Lewandowski measure [20], which defines the Hilbert space $\mathcal{H} = L^2(\bar{\mathcal{A}}, \mathrm{d}\mu_{\mathrm{AL}})$ of square integrable functions on the space of generalized connections. A dense subset Cyl of functions is given by cylindrical functions $f(h_{e_1}, \ldots, h_{e_n})$, which depend on the connection through a finite but arbitrary number of holonomies. These cylindrical functions are associated with graphs g formed by the edges e_1, $\ldots$, e_n. For functions cylindrical with respect to two identical graphs the inner product can be written as

$$\langle f|g\rangle = \int_{\bar{\mathcal{A}}} \mathrm{d}\mu_{\mathrm{AL}}(A) f(A)^* g(A) = \int_{\mathrm{SU}(2)^n} \prod_{i=1}^{n} \mathrm{d}\mu_{\mathrm{H}}(h_i) f(h_1,\ldots,h_n)^* g(h_1,\ldots,h_n), \qquad (10)$$

with the Haar measure $\mathrm{d}\mu_{\mathrm{H}}$ on G. The importance of generalized connections can be seen from the fact that the space $\mathcal{A}$ of smooth connections is a subset of measure zero in $\bar{\mathcal{A}}$ [224].

With the dense subset Cyl of $\mathcal{H}$ we obtain the Gel'fand triple

$$\mathrm{Cyl} \subset \mathcal{H} \subset \mathrm{Cyl}^* \qquad (11)$$

with the dual Cyl^* of linear functionals from Cyl to the set of complex numbers. Elements of Cyl^* are distributions, and there is no inner product on the full space. However, one can define inner products on certain subspaces defined by the physical context. Often, those subspaces appear when constraints with continuous spectra are solved following the Dirac procedure. Other examples include the definition of semiclassical or, as we will use it in Section 7, symmetric states.

3.5 Composite operators

From the basic operators we can construct more complicated ones which, with growing degrees of complexity, will be more and more ambiguous for, example from factor ordering choices. Quite simple expressions exist for the area and volume operator [260, 21, 22], which are constructed solely from fluxes. Thus, they are less ambiguous, since no factor-ordering issues with holonomies arise. This is true because the area of a surface and volume of a region can be written classically as functionals of the densitized triad alone, $A_S = \int_S \sqrt{E^a_i n_a E^b_i n_b}\mathrm{d}^2y$ and $V_R = \int_R \sqrt{|\det E^a_i|}\mathrm{d}^3x$. At the quantum level this implies that, like fluxes, area and volume also have discrete spectra, showing that spatial quantum geometry is discrete. (For discrete approaches to quantum gravity in general see [218].) All area eigenvalues are known explicitly, but this is not possible, even in principle, for the volume operator. Nevertheless, some closed formulas and numerical techniques exist [217, 150, 149, 118].

The length of a curve, on the other hand, requires the co-triad, which is an inverse of the densitized triad and is more problematic. Since fluxes have discrete spectra containing zero, they do not have densely defined inverse operators. As we will describe below, it is possible to quantize those expressions, but it requires one to use holonomies. Thus, we encounter here more ambiguities from factor ordering. Still, one can show that length operators also have discrete spectra [290].

Inverse-densitized triad components also arise when we try to quantize matter Hamiltonians, such as

$$H_\phi = \int \mathrm{d}^3x \left(\frac{1}{2} \frac{p_\phi^2 + E^a_i E^b_i \partial_a\phi \partial_b\phi}{\sqrt{|\det E^c_j|}} + \sqrt{|\det E^c_j|} V(\phi) \right), \qquad (12)$$

for a scalar field ϕ with momentum p_ϕ and potential $V(\phi)$ (not to be confused with volume). The inverse determinant again cannot be quantized directly by using, e.g., an inverse of the volume operator, which does not exist. This seems, at first, to be a severe problem, not unlike the situation in quantum field theory on a background where matter Hamiltonians are divergent. Yet it turns out that quantum geometry allows one to quantize these expressions in a well-defined manner [291].

To do this, we notice that the Poisson bracket of the volume with connection components,

$$\{A^i_a, \int \sqrt{|\det E|}\mathrm{d}^3x\} = 2\pi\gamma G \epsilon^{ijk} \epsilon_{abc} \frac{E^b_j E^c_k}{\sqrt{|\det E|}}, \qquad (13)$$

amounts to an inverse of densitized triad components and allows a well-defined quantization: we can express the connection component through holonomies, use the volume operator and turn the Poisson bracket into a commutator. Since all operators involved have a dense intersection of their domains of definition, the resulting operator is densely defined and provides a quantization of inverse powers of the densitized triad.

This also shows that connection components or holonomies are required in this process and, thus, ambiguities can arise, even if initially one starts with an expression such as $\sqrt{|\det E|}^{-1}$, which only depends on the triad. There are also many different ways to rewrite expressions as above, which all are equivalent classically but result in different quantizations. In classical regimes this would not be relevant, but can have sizeable effects at small scales. In fact, this particular aspect, which as a general mechanism is a direct consequence of the background-independent quantization with its discrete fluxes, implies characteristic modifications of the classical expressions on small scales. We will discuss this and more detailed examples in the cosmological context in Section 4.

3.6 Hamiltonian constraint

Similarly to matter Hamiltonians one can also quantize the Hamiltonian constraint in a well-defined manner [292]. Again, this requires us to rewrite triad components and to make other regularization choices. Thus, there is not just one quantization but a class of different possibilities.

It is more direct to quantize the first part of the constraint containing only the Ashtekar curvature. (This part agrees with the constraint in Euclidean signature and Barbero–Immirzi parameter $\gamma = 1$, and so is sometimes called the Euclidean part of the constraint.) Triad components and their inverse determinant are again expressed as a Poisson bracket using identity (13), and curvature components are obtained through a holonomy around a small loop α of coordinate size Δ and with tangent vectors s_1^a and s_2^a at its base point [259]:

$$s_1^a s_2^b F_{ab}^i \tau_i = \Delta^{-1}(h_\alpha - 1) + O(\Delta)\,. \tag{14}$$

Putting this together, an expression for the Euclidean part $H^{\mathrm{E}}[N]$ can then be constructed in the schematic form

$$H^{\mathrm{E}}[N] \propto \sum_v N(v)\epsilon^{IJK}\mathrm{tr}\left(h_{\alpha_{IJ}} h_{s_K}\{h_{s_K}^{-1}, V\}\right) + O(\Delta), \tag{15}$$

where one sums over all vertices of a triangulation of space, whose tetrahedra are used to define closed curves α_{IJ} and transversal edges s_K.

An important property of this construction is that coordinate functions such as Δ disappear from the leading term, such that the coordinate size of the discretization is irrelevant. Nevertheless, there are several choices to be made, such as how a discretization is chosen in relation to the graph a constructed operator is supposed to act on, which in later steps will have to be constrained by studying properties of the quantization. Of particular interest is the holonomy h_α, since it creates new edges to a graph, or at least new spin on existing ones. Its precise behavior is expected to have a strong influence on the resulting dynamics [283]. In addition, there are factor-ordering choices, i.e., whether triad components appear to the right or left of curvature components. It turns out that the expression above leads to a well-defined operator only in the first case, which, in particular, requires an operator non-symmetric in the kinematical inner product. Nevertheless, one can always take that operator and add its adjoint (which in this full setting does not simply amount to reversing the order of the curvature and triad expressions) to obtain a symmetric version, such that the choice still exists. Another choice is the representation chosen to take the trace, which for this construction is not required to be the fundamental one [170].

The second part of the constraint is more complicated since one has to use the function $\Gamma(E)$ in K_a^i. As also developed in [292], extrinsic curvature can be obtained through the already-constructed Euclidean part via $K \sim \{H^{\mathrm{E}}, V\}$. The result, however, is rather complicated, and in models one often uses a more direct way, exploiting the fact that Γ has a more special form. In this way, additional commutators in the general construction can be avoided, which usually does not have strong effects. Sometimes, however, these additional commutators can be relevant, which may always be determined by a direct comparison of different constructions (see, e.g., [181]).

3.7 Relational dynamics

The typical form of Hamiltonian constraint operators in loop quantum gravity following [259, 292] prevents single-spin network states from being physical, i.e., annihilated by the constraint operator. As a consequence of the creation of new edges and vertices by the constraint, physical states cannot be based on a single graph but must be superpositions of different graph states. Such superpositions can be complicated, but generally they can be understood as encoding the relational dynamics of gravity in the absence of an absolute time. Rather than using an external time coordinate one chooses an internal time variable from the dynamical fields. In general situations, no global time exists but locally evolution can be described in suitable variables. Especially in cosmology it is often convenient to use the spatial volume as internal time and thus, at least formally, expand a state in volume eigenstates. Since each action of the Hamiltonian constraint changes spins and the graph, and thus the volume, its basic action can be seen to provide elementary moves of a dynamically changing lattice (see [73] for more details). Typically, larger volumes require finer graphs and thus the underlying lattice is refined as the universe expands. New degrees of freedom emerge while the universe grows, which is a characteristic feature of quantum gravity.

In the full theory, finding solutions and decomposing them in volume eigenstates is currently out of reach. But qualitative aspects of this process can be incorporated in models as described in the following. The models, in turn, can often be analyzed much more easily and thus allow crucial tests of the general framework. Several non-trivial consistency checks have by now been performed and given valuable insights into the dynamics of loop quantum gravity.

3.8 Open issues

For an anomaly-free quantization the constraint operators have to satisfy an algebra mimicking the classical one. There are arguments that this is the case for quantization as described above, when each loop α contains exactly one vertex of a given graph [288], but the issue is still open. Moreover, the operators are quite complicated and it is not easy to see if they have the correct expectation values in appropriately defined semiclassical states.

Even if one regards the quantization and semiclassical issues as satisfactory, one has to face several hurdles in evaluating the theory. There are interpretational issues of the wave function obtained as a solution to the constraints, and the problem of time or observables emerges as well [209]. There is a wild mixture of conceptual and technical problems at different levels, not least because the operators are quite complicated. For instance, as seen in the rewriting procedure above, the volume operator plays an important role, even if one is not necessarily interested in the volume of regions. Since this operator is complicated, without an explicitly known spectrum it translates to complicated matrix elements of the constraints and matter Hamiltonians. Loop quantum gravity should thus be considered as a framework rather than a uniquely defined theory, which, however, has important rigid aspects. This includes the basic representation of the holonomy-flux algebra and its general consequences.

All this should not come as a surprise since even classical gravity, at this level of generality, is complicated enough. Most solutions and results in general relativity are obtained with approximations or assumptions, one of the most widely used being symmetry reduction. In fact, this allows access to the most interesting gravitational phenomena such as cosmological expansion, black holes and gravitational waves. Similarly, symmetry reduction is expected to simplify many problems of full quantum gravity by resulting in simpler operators and by isolating conceptual problems such that not all of them need to be considered at once. By systematic perturbation expansions around symmetric models, the crucial physical issues facing loop quantum gravity can be analyzed without restricting the number of degrees of freedom.

4 Loop Cosmology

Je abstrakter die Wahrheit ist, die du lehren willst, um so mehr mußt du noch die Sinne zu ihr verführen.

(*The more abstract the truth you want to teach is, the more you have to seduce to it the senses.*)

Friedrich Nietzsche
Beyond Good and Evil

The gravitational field equations, for instance in the case of cosmology where one can assume homogeneity and isotropy, involve components of curvature as well as the inverse metric. (Computational methods to derive information from these equations are described in [5].) Since singularities occur, these curvature components become large in certain regimes, but the equations have been tested only in small curvature regimes. On small length scales, such as close to the Big Bang, modifications to the classical equations are not ruled out by observations and can be expected from candidates of quantum gravity. Quantum cosmology describes the evolution of a universe by a constraint equation for a wave function, but some effects can be included already at the level of effective classical equations. In loop quantum gravity one characteristic quantum correction occurs through inverse metric components, which, e.g., appear in the kinematic term of matter Hamiltonians; see Section 4.4. In addition, holonomies provide higher powers of connection components and thus additional effects in the dynamics as described in Section 4.7. While the latter dominate in many homogeneous models, which have been analyzed in detail, this is a consequence of the homogeneity assumption. More generally, effects from inverse metric components play equally important roles and are currently under better control, e.g., regarding the anomaly issue (see Section 6.5.4).

4.1 Isotropy

Isotropy reduces the phase space of general relativity to two-dimensions since, up to SU(2)-gauge freedom, there is only one independent component in an isotropic connection and triad, which is not already determined by the symmetry. This is analogous to metric variables, where the scale factor a is the only free component in the spatial part of an isotropic metric

$$\mathrm{d}s^2 = -N(t)^2\,\mathrm{d}t^2 + a(t)^2((1-kr^2)^{-1}\,\mathrm{d}r^2 + r^2\,\mathrm{d}\Omega^2)\,. \tag{16}$$

The lapse function $N(t)$ does not play a dynamical role and correspondingly does not appear in the Friedmann equation

$$\left(\frac{\dot a}{a}\right)^2 + \frac{k}{a^2} = \frac{8\pi G}{3} a^{-3} H_{\mathrm{matter}}(a) \tag{17}$$

where H_{matter} is the matter Hamiltonian, G is the gravitational constant, and the parameter k takes the discrete values zero or ± 1 depending on the symmetry group or intrinsic spatial curvature.

Indeed, $N(t)$ can simply be absorbed into the time coordinate by defining proper time τ through $\mathrm{d}\tau = N(t)\mathrm{d}t$. This is not possible for the scale factor since it depends on time but multiplies space differentials in the line element. The scale factor can only be rescaled by an arbitrary constant, which can be normalized, at least in the closed model where $k = 1$.

One can also understand these different roles of metric components from a Hamiltonian analysis of the Einstein–Hilbert action

$$S_{\mathrm{EH}} = \frac{1}{16\pi G}\int \mathrm{d}t\,\mathrm{d}^3x R[g]$$

specialized to isotropic metrics (16), whose Ricci scalar is

$$R = 6\left(\frac{\ddot{a}}{N^2 a} + \frac{\dot{a}^2}{N^2 a^2} + \frac{k}{a^2} - \frac{\dot{a}}{a}\frac{\dot{N}}{N^3}\right).$$

The action then becomes

$$S = \frac{V_0}{16\pi G}\int \mathrm{d}t\, N a^3 R = \frac{3V_0}{8\pi G}\int \mathrm{d}t\, N\left(-\frac{a\dot{a}^2}{N^2} + ka\right)$$

(with the spatial coordinate volume $V_0 = \int_\Sigma \mathrm{d}^3x$) after integrating by parts, from which one derives the momenta

$$p_a = \frac{\partial L}{\partial \dot{a}} = -\frac{3V_0}{4\pi G}\frac{a\dot{a}}{N} \quad , \quad p_N = \frac{\partial L}{\partial \dot{N}} = 0$$

illustrating the different roles of a and N. Since p_N must vanish, N is not a degree of freedom but a Lagrange multiplier. It appears in the canonical action $S = (16\pi G)^{-1}\int \mathrm{d}t(\dot{a}p_a - NH))$ only as a factor of

$$H_{\mathrm{ADM}} = -\frac{2\pi G}{3}\frac{p_a^2}{V_0 a} - \frac{3}{8\pi G}V_0 a k, \tag{18}$$

such that variation with respect to N forces H, the Hamiltonian constraint, to be zero. In the presence of matter, H also contains the matter Hamiltonian, and its vanishing is equivalent to the Friedmann equation.

4.2 Isotropy: Connection variables

Isotropic connections and triads, as discussed in Appendix B.2, are analogously described by single components $\tilde{c}$ and $\tilde{p}$, respectively, related to the scale factor by

$$|\tilde{p}| = \tilde{a}^2 = \frac{a^2}{4} \tag{19}$$

for the densitized triad component $\tilde{p}$ and

$$\tilde{c} = \tilde{\Gamma} + \gamma\dot{\tilde{a}} = \frac{1}{2}(k + \gamma\dot{a}) \tag{20}$$

for the connection component $\tilde{c}$. Both components are canonically conjugate:

$$\{\tilde{c}, \tilde{p}\} = \frac{8\pi\gamma G}{3V_0}. \tag{21}$$

It is convenient to absorb factors of V_0 into the basic variables, which is also suggested by the integrations in holonomies and fluxes on which background-independent quantizations are built [16]. We thus define

$$p = V_0^{2/3}\tilde{p}, \qquad c = V_0^{1/3}\tilde{c} \tag{22}$$

together with $\Gamma = V_0^{1/3}\tilde{\Gamma}$. The symplectic structure is then independent of V_0 and so are integrated densities such as total Hamiltonians. For the Hamiltonian constraint in isotropic Ashtekar variables we have

$$H = -\frac{3}{8\pi G}(\gamma^{-2}(c-\Gamma)^2 + \Gamma^2)\sqrt{|p|} + H_{\mathrm{matter}}(p) = 0, \tag{23}$$

which is exactly the Friedmann equation. (In most earlier papers on loop quantum cosmology some factors in the basic variables and classical equations are incorrect due, in part, to the existence of different and often confusing notation in the loop quantum gravity literature.[1] Note that H here seems to differ from H_{ADM} in (18) by a factor of 8. This happens due to different normalizations of the coordinate volume V_0, which is a unit 3-sphere for a closed model in Friedmann–Robertson–Walker form, while isotropic connection variables, as reduced in Appendix B.2, are based on a 2-fold covering space obtained from isotropizing a Bianchi IX model.)

The part of phase space where we have $p = 0$ and thus $a = 0$ plays a special role since this is where isotropic classical singularities are located. On this subset the evolution equation (17) with standard matter choices is singular in the sense that H_{matter}, e.g.,

$$H_\phi(a, \phi, p_\phi) = \frac{1}{2}|p|^{-3/2}p_\phi^2 + |p|^{3/2}V(\phi) \tag{24}$$

for a scalar ϕ with momentum p_ϕ and potential $V(\phi)$, diverges and the differential equation does not pose a well-defined initial-value problem there. Thus, once such a point is reached, the further evolution is no longer determined by the theory. Since, according to singularity theorems [178, 114], any classical trajectory must intersect the subset $a = 0$ for the matter we need in our universe, the classical theory is incomplete.

This situation, certainly, is not changed by introducing triad variables instead of metric variables. However, the situation is already different since $p = 0$ is a sub-manifold in the classical phase space of triad variables, where p can have both signs (the sign determining whether the triad is left or right handed, i.e., the orientation). This is in contrast to metric variables where $a = 0$ is a boundary of the classical phase space. There are no implications in the classical theory since trajectories end there anyway, but it will have important ramifications in the quantum theory (see Sections 5.14, **??**, 5.17 and 5.19).

4.3 Isotropy: Implications of a loop quantization

We are now dealing with a simple system with finitely many degrees of freedom, subject to a constraint. It is well known how to quantize such a system from quantum mechanics, which has been applied to cosmology starting with DeWitt [152]. Here one chooses a metric representation for wave functions, i.e., $\psi(a)$, on which the scale factor acts as a multiplication operator and its conjugate p_a, related to $\dot{a}$, as a derivative operator. These basic operators are then used to form the Wheeler–DeWitt operator quantizing the constraint (17) once a factor ordering is chosen.

This prescription is rooted in quantum mechanics, which, despite its formal similarity, is physically very different from cosmology. The procedure looks innocent, but one should realize that there are already basic choices involved. Choosing the factor ordering is harmless, even though results can depend on it [206]. More importantly, one has chosen the Schrödinger representation of the classical Poisson algebra, which immediately implies the familiar properties of operators such as the scale factor with a continuous spectrum. There are inequivalent representations with different properties, and it is not clear that this representation, which works well in quantum mechanics, is also correct for quantum cosmology. In fact, quantum mechanics is not very sensitive to the representation chosen [19] and one can use the most convenient one. This is the case because energies and thus oscillation lengths of wave functions, described usually by quantum mechanics, span only a limited range. Results can then be reproduced to arbitrary accuracy in any representation. Quantum cosmology, in contrast, has to deal with potentially infinitely-high matter energies, leading to small oscillation lengths of wave functions, such that the issue of quantum representations becomes essential.

That the Wheeler–DeWitt representation may not be the right choice is also indicated by the fact that its scale factor operator has a continuous spectrum, while quantum geometry, which

[1] The author is grateful to Ghanashyam Date and Golam Hossain for discussions and correspondence on this issue.

at least kinematically is a well-defined quantization of the full theory, implies discrete volume spectra. Indeed, the Wheeler–DeWitt quantization of full gravity exists only formally, and its application to quantum cosmology simply quantizes the classically-reduced isotropic system. This is much easier, and also more ambiguous, and leaves open many consistency considerations. It would be more reliable to start with the full quantization and introduce the symmetries there, or at least follow the same constructions of the full theory in a reduced model. If this is done, it turns out that indeed we obtain a quantum representation inequivalent to the Wheeler–DeWitt representation, with strong implications in high-energy regimes. In particular, like the full theory, such a quantization has a volume or p operator with a discrete spectrum, as derived in Section 5.2.

4.4 Isotropy: Effective densities in phenomenological equations

The isotropic model is thus quantized in such a way that the operator $\hat{p}$ has a discrete spectrum containing zero. This immediately leads to a problem, since we need a quantization of $|p|^{-3/2}$ in order to quantize a matter Hamiltonian such as (24), where not only the matter fields but also the geometry is quantized. However, an operator with zero in the discrete part of its spectrum does not have a densely defined inverse and does not allow a direct quantization of $|p|^{-3/2}$.

This leads us to the first main effect of the loop quantization: It turns out that despite the non-existence of an inverse operator of $\hat{p}$ one can quantize the classical $|p|^{-3/2}$ to a well-defined operator. This is not just possible in the model but also in the full theory, where it has even been defined first [291]. Classically, one can always write expressions in many equivalent ways, which usually results in different quantizations. In the case of $|p|^{-3/2}$, as discussed in Section 5.3, there is a general class of ways to rewrite it in a quantizable manner [49], which differ in details but all have the same important properties. This can be parameterized by a function $d(p)_{j,l}$ [55, 58], which replaces the classical $|p|^{-3/2}$ and strongly deviates from it for small p, while being very close at large p. The parameters $j \in \frac{1}{2}\mathbb{N}$ and $0 < l < 1$ specify quantization ambiguities resulting from different ways of rewriting. With the function

$$p_l(q) = \frac{3}{2l} q^{1-l} \left(\frac{1}{l+2} \left((q+1)^{l+2} - |q-1|^{l+2} \right) - \frac{1}{l+1} q \left((q+1)^{l+1} - \operatorname{sgn}(q-1)|q-1|^{l+1} \right) \right) \tag{25}$$

we have

$$d(p)_{j,l} := |p|^{-3/2} p_l (3|p|/\gamma j \ell_{\mathrm{P}}^2)^{3/(2-2l)}, \tag{26}$$

which indeed fulfills $d(p)_{j,l} \sim |p|^{-3/2}$ for $|p| \gg p_* := \frac{1}{3} j \gamma \ell_{\mathrm{P}}^2$, but is finite with a peak around p_* and approaches zero at $p = 0$ in a manner

$$d(p)_{j,l} \sim 3^{3(3-l)/(2-2l)} (l+1)^{-3/(2-2l)} (\gamma j)^{-3(2-l)/(2-2l)} \ell_{\mathrm{P}}^{-3(2-l)/(1-l)} |p|^{3/(2-2l)} \tag{27}$$

as it follows from $p_l(q) \sim 3q^{2-l}/(1+l)$. Some examples displaying characteristic properties are shown in Figure 9 in Section 5.3.

The matter Hamiltonian obtained in this manner will thus behave differently at small p. At those scales other quantum effects such as fluctuations can also be important, but it is possible to isolate the effect implied by the modified density (26). We just need to choose a rather large value for the ambiguity parameter j, such that modifications become noticeable even in semiclassical regimes. This is mainly a technical tool to study the behavior of equations, but can also be used to find constraints on the allowed values of ambiguity parameters.

We can thus use classical equations of motion, which are corrected for quantum effects by using the phenomenological matter Hamiltonian

$$H_\phi^{(\mathrm{phen})}(p, \phi, p_\phi) := \frac{1}{2} d(p)_{j,l} p_\phi^2 + |p|^{3/2} V(\phi) \tag{28}$$

(see Section 6 for details on the relationship to effective equations). This matter Hamiltonian changes the classical constraint such that now

$$H = -\frac{3}{8\pi G}(\gamma^{-2}(c-\Gamma)^2+\Gamma^2)\sqrt{|p|} + H_\phi^{(\mathrm{phen})}(p,\phi,p_\phi) = 0\,. \tag{29}$$

Since the constraint determines all equations of motion, they also change; we obtain the Friedmann equation from $H = 0$,

$$\left(\frac{\dot a}{a}\right)^2 + \frac{k}{a^2} = \frac{8\pi G}{3}\left(\frac{1}{2}|p|^{-3/2}d(p)_{j,l}p_\phi^2 + V(\phi)\right) \tag{30}$$

and the Raychaudhuri equation from $\dot c = \{c, H\}$,

$$\frac{\ddot a}{a} = -\frac{4\pi G}{3|p|^{3/2}}\left(H_{\mathrm{matter}}(p,\phi,p_\phi) - 2p\frac{\partial H_{\mathrm{matter}}(p,\phi,p_\phi)}{\partial p}\right) \tag{31}$$

$$= -\frac{8\pi G}{3}\left(|p|^{-3/2}d(p)_{j,l}^{-1}\dot\phi^2\left(1-\tfrac{1}{4}a\frac{\mathrm{d}\log(|p|^{3/2}d(p)_{j,l})}{\mathrm{d}a}\right) - V(\phi)\right). \tag{32}$$

Matter equations of motion follow similarly as

$$\dot\phi = \{\phi, H\} = d(p)_{j,l}p_\phi$$
$$\dot p_\phi = \{p_\phi, H\} = -|p|^{3/2}V'(\phi),$$

which can be combined to form the Klein–Gordon equation

$$\ddot\phi = \dot\phi\,\dot a\frac{\mathrm{d}\log d(p)_{j,l}}{\mathrm{d}a} - |p|^{3/2}d(p)_{j,l}V'(\phi)\,. \tag{33}$$

4.5 Isotropy: Properties and intuitive meaning of effective densities

As a consequence of the function $d(p)_{j,l}$, the phenomenological equations have different qualitative behavior at small versus large scales p. In the Friedmann equation (30) this is most easily seen by comparing it with a mechanics problem with a standard Hamiltonian, or energy, of the form

$$E = \frac{1}{2}\dot a^2 - \frac{2\pi G}{3V_0}a^{-1}d(p)_{j,l}p_\phi^2 - \frac{4\pi G}{3}a^2V(\phi) = 0$$

that is restricted to be zero. If we assume a constant scalar potential $V(\phi)$, there is no ϕ-dependence and the scalar equations of motion show that p_ϕ is constant. Thus, the potential for the motion of a is essentially determined by the function $d(p)_{j,l}$.

In the classical case, $d(p) = |p|^{-3/2}$ and the potential is negative and increasing, with a divergence at $p = 0$. The scale factor a is thus driven toward $a = 0$, which it will always reach in finite time where the system breaks down. With the effective density $d(p)_{j,l}$, however, the potential is bounded from below, and is decreasing from zero for $a = 0$ to the minimum around p_*. Thus, the scale factor is now slowed down before it reaches $a = 0$, which, depending on the matter content, could avoid the classical singularity altogether.

The behavior of matter is also different as shown by the Klein–Gordon equation (33). Most importantly, the derivative in the $\dot\phi$-term changes sign at small a since the effective density is increasing there. Thus, the qualitative behavior of all the equations changes at small scales, which, as we will see, gives rise to many characteristic effects. Nevertheless, for the analysis of the equations, as well as for conceptual considerations, it is interesting that solutions at small and large scales are connected by a duality transformation [214, 132], which even exists between effective solutions for loop cosmology and braneworld cosmology [133].

We have seen that the equations of motion following from a phenomenological Hamiltonian incorporating effective densities are expected to display qualitatively different behavior at small scales. Before discussing specific models in detail, it is helpful to observe what physical meaning the resulting modifications have.

Classical gravity is always attractive, which implies that there is nothing to prevent collapse in black holes or the whole universe. In the Friedmann equation this is expressed by the fact that the potential, as used before, is always decreasing toward $a = 0$, where it diverges. With the effective density, on the other hand, we have seen that the decrease stops and instead the potential starts to increase at a certain scale before it reaches zero at $a = 0$. This means that at small scales, where quantum gravity becomes important, the gravitational attraction turns into repulsion. In contrast to classical gravity, thus, quantum gravity has a repulsive component, which can potentially prevent collapse. So far, this has only been demonstrated in homogeneous models, but it relies on a general mechanism which is also present in the full theory.

Not only the attractive nature of gravity changes at small scales, but also the behavior of matter in a gravitational background. Classically, matter fields in an expanding universe are slowed down by a friction term in the Klein–Gordon equation (33), where $\dot{a}\mathrm{d}\log a^{-3}/\mathrm{d}a = -3\dot{a}/a$ is negative. Conversely, in a contracting universe matter fields are excited and even diverge when the classical singularity is reached. This behavior turns around at small scales, where the derivative $\mathrm{d}\log d(a)_{j,l}/\mathrm{d}a$ becomes positive. Friction in an expanding universe then turns into antifriction such that matter fields are driven away from their potential minima before classical behavior sets in. In a contracting universe, on the other hand, matter fields are not excited by antifriction but freeze once the universe becomes small enough.

These effects do not only have implications for the avoidance of singularities at $a = 0$ but also for the behavior at small but non-zero scales. Gravitational repulsion can not only prevent the collapse of a contracting universe [279] but also, in an expanding universe, enhance its expansion. The universe then accelerates in an inflationary manner from quantum gravity effects alone [53]. Similarly, the new behavior of matter fields has implications for inflationary models [111].

4.6 Isotropy: Applications of effective densities

There is now one characteristic correction of the matter Hamiltonian, coming directly from a loop quantization. Its implications can be interpreted as repulsive behavior on small scales and the exchange of friction and antifriction for matter, and it leads to many further consequences.

4.6.1 Collapsing phase

When the universe has collapsed to a sufficiently small size, repulsion becomes noticeable and bouncing solutions become possible, as illustrated in Figure 1. Requirements for a bounce are that the conditions $\dot{a} = 0$ and $\ddot{a} > 0$ can be fulfilled at the same time, where the first can be evaluated with the Friedmann equation and the second with the Raychaudhuri equation. The first condition can only be fulfilled if there is a negative contribution to the matter energy, which can come from a positive curvature term $k = 1$ or a negative matter potential $V(\phi) < 0$. In these cases, there are classical solutions with $\dot{a} = 0$, but they generically have $\ddot{a} < 0$ corresponding to a recollapse. This can easily be seen in the flat case with a negative potential, where Equation (31) is strictly negative with $\mathrm{d}\log a^3 d(a)_{j,l}/\mathrm{d}a \approx 0$ at large scales.

The repulsive nature at small scales now implies a second point where $\dot{a} = 0$ from Equation (30) at smaller a since the matter energy now also decreases as $a \to 0$. Moreover, the Raychaudhuri equation (31) has an additional positive term at small scales such that $\ddot{a} > 0$ becomes possible.

Matter also behaves differently through the Klein–Gordon equation (33). Classically, with $\dot{a} < 0$, the scalar experiences antifriction and ϕ diverges close to the classical singularity. With the quantum correction, antifriction turns into friction at small scales, damping the motion of ϕ such that it remains finite. In the case of a negative potential [98], this allows the kinetic term to cancel the potential term in the Friedmann equation. With a positive potential and positive curvature, on the other hand, the scalar is frozen and the potential is canceled by the curvature term. Since the scalar is almost constant, the behavior around the turning point is similar to a de Sitter bounce [279, 303]. Further, more generic possibilities for bounces arise from other correction terms [147, 142].

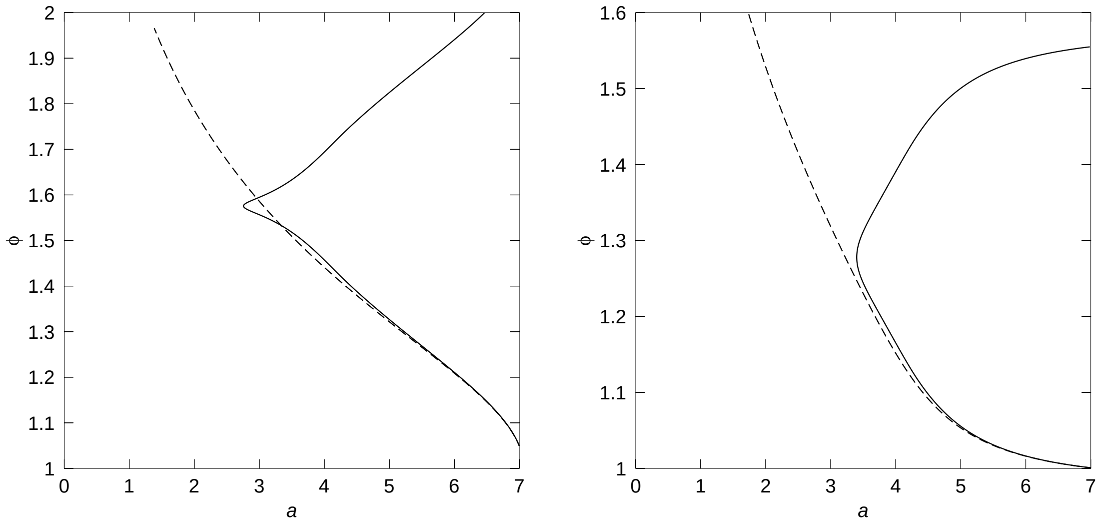

Figure 1: Examples of bouncing solutions with positive curvature (left) or a negative potential (right, negative cosmological constant). The solid lines show solutions of equations with a bounce as a consequence of quantum corrections, while the dashed lines show classical solutions running into the singularity at $a = 0$ where ϕ diverges.

4.6.2 Expansion

Repulsion can not only prevent collapse but also accelerates an expanding phase. Indeed, using the behavior (27) at small scales in the Raychaudhuri equation (31) shows that $\ddot{a}$ is generically positive since the inner bracket is smaller than $-1/2$ for the allowed values $0 < l < 1$. Thus, as illustrated by the numerical solution in the upper left panel of Figure 2, inflation is realized by quantum gravity effects for any matter field irrespective of its form, potential or initial values [53]. The kind of expansion at early stages is generally super-inflationary, i.e., with equation of state parameter $w < -1$. For free massless matter fields, w usually starts very small, depending on the value of l, but with a non-zero potential just as the mass term for matter inflation w is generally close to exponential: $w_{\mathrm{eff}} \approx -1$ for small p. This can be shown by a simple and elegant argument independently of the precise matter dynamics [148]; the equation of state parameter is defined as $w = P/\rho$ where $P = -\partial E/\partial V$ is the pressure, i.e., the negative change of energy with respect to volume, and $\rho = E/V$ is the energy density. Using the matter Hamiltonian for E and $V = |p|^{3/2}$, we obtain

$$P_{\mathrm{eff}} = -\tfrac{1}{3}|p|^{-1/2} d'(p) p_\phi^2 - V(\phi)$$

and thus, in the classical case,

$$w = \frac{\frac{1}{2}|p|^{-3}p_\phi^2 - V(\phi)}{\frac{1}{2}|p|^{-3}p_\phi^2 + V(\phi)}$$

as usual. In loop cosmology, however, we have

$$w_{\mathrm{eff}} = -\frac{\frac{1}{3}|p|^{-1/2}d'(p)p_\phi^2 + V(\phi)}{\frac{1}{2}|p|^{-3/2}d(p)p_\phi^2 + V(\phi)}\,.$$

(See [312] for a discussion of energy conditions in this context and [272] for an application to tachyon fields.)

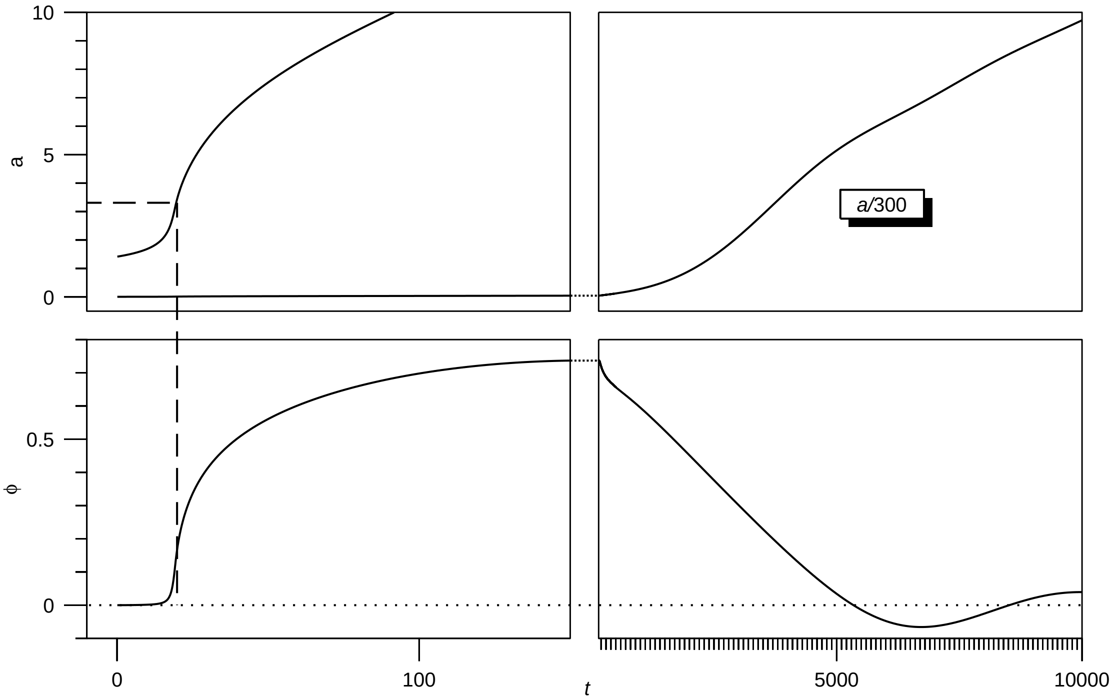

Figure 2: Example of a solution of $a(t)$ and $\phi(t)$ showing early loop inflation and later slow-roll inflation driven by a scalar that has pushed up its potential by loop effects. The left-hand side is stretched in time so as to show all details. An idea of the duration of different phases can be obtained from Figure 3.

In general we need to know the matter behavior to know w and w_{eff}. But we can get general qualitative information by treating p_ϕ and $V(\phi)$ as unknowns determined by w and w_{eff}. In the general case there is no unique solution for p_ϕ^2 and $V(\phi)$ since, after all, p_ϕ and ϕ change with t. They are now subject to two linear equations in terms of w and w_{eff}, whose determinant must be zero, resulting in

$$w_{\mathrm{eff}} = -1 + \frac{|p|^{3/2}(w+1)(d(p) - \frac{2}{3}|p|d'(p))}{1 - w + (w+1)|p|^{3/2}d(p)}\,.$$

Since for small p the numerator of the fraction approaches zero faster than the second part of the denominator, w_{eff} approaches -1 at small volume except for the special case where $w = 1$, which is realized for $V(\phi) = 0$. Note that the argument does not apply to the case of vanishing potential since then $p_\phi^2 = \mathrm{const}$ and $V(\phi) = 0$ presents a unique solution to the linear equations for w and w_{eff}.

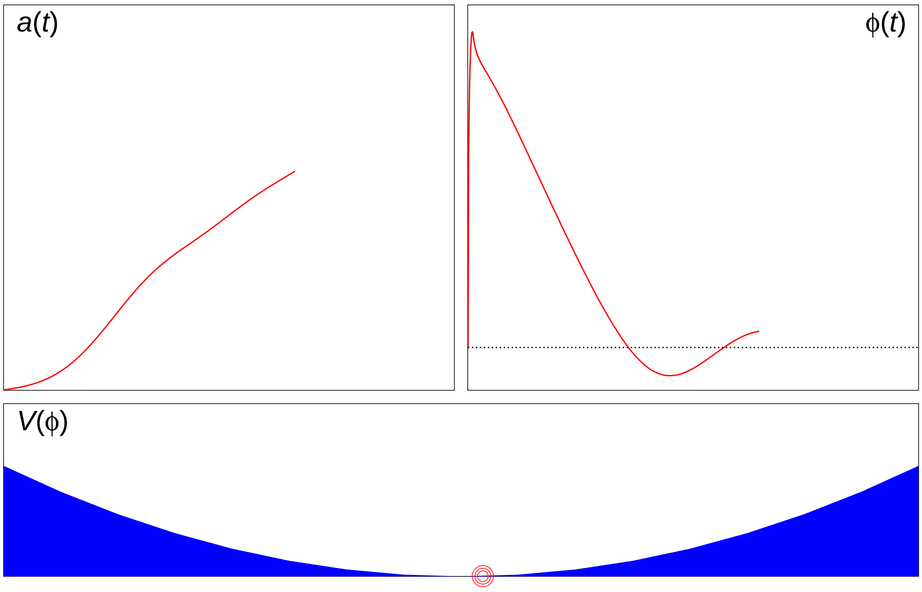

Figure 3: Still from a movie showing The initial push of a scalar ϕ up its potential and the ensuing slow-roll phase together with the corresponding inflationary phase of a. (To watch the movie, please go to the online version of this review article at `http://www.livingreviews.org/lrr-2008-4`.)

In fact, this case leads in general to a much smaller $w_{\rm eff} = -\frac{2}{3}|p|d(p)'/d(p) \approx -1/(1-l) < -1$ [53]. Also at intermediate values of p, where the asymptotic argument does not apply, values of $w_{\rm eff}$ that are smaller than -1 are possible.

One can also see from the above formula that $w_{\rm eff}$, though close to -1, is a little smaller than -1 generally. This is in contrast to single field inflaton models where the equation of state parameter is a little larger than -1. As we will discuss in Section 4.19, this opens the door to possible characteristic signatures distinguishing different models. However, here we refer to a regime where other quantum corrections are present and care in the interpretation of results is thus required.

Again, the matter behavior also changes, now with classical friction being replaced by antifriction [111]. Matter fields thus move away from their minima and become excited, even if they start close to a minimum (Figure 2). Since this does not apply only to the homogeneous mode, it can provide a mechanism for structure formation as discussed in Section 4.19. But modified matter behavior also leads to improvements in combination with chaotic inflation as the mechanism to generate structure; if we now view the scalar ϕ as an inflaton field, it will be driven to large values in order to start a second phase of slow-roll inflation that is long enough. This "graceful entrance" [244] is satisfied for a large range of the ambiguity parameters j and l [97] (see also [195]), is insensitive to non-minimal coupling of the scalar [93], and can even leave signatures [295] in the cosmic microwave spectrum [194]. The earliest moments during which the inflaton starts to roll down its potential are not slow roll, as can also be seen in Figures 2 and 3, where the initial decrease is steeper. Provided the resulting structure can be seen today, i.e., there are not too many e-foldings from the second phase, this can lead to visible effects, such as a suppression of power. Whether or not those effects are to be expected, i.e., which magnitude of the inflaton is generally reached by the mechanism generating initial conditions, is to be investigated at the basic level of loop quantum cosmology. All this should be regarded only as initial suggestions, indicating the potential of quantum cosmological phenomenology, which have to be substantiated by detailed calculations, including inhomogeneities or at least anisotropic geometries. In particular, the suppression of power can be obtained by a multitude of other mechanisms.

4.6.3 Model building

It is already clear that there are different inflationary scenarios using effects from loop cosmology. A scenario without inflatons is more attractive since it requires less choices and provides a fundamental explanation for inflation directly from quantum gravity. However, it is also more difficult to analyze structure formation in this context, when there already are well-developed techniques in slow role scenarios.

In these cases, where one couples loop cosmology to an inflaton model, one still requires the same conditions for the potential, but generally gets the required large initial values for the scalar by antifriction. On the other hand, finer details of the results now depend on the ambiguity parameters, which describe aspects of the quantization also arising in the full theory.

It is possible to combine collapsing and expanding phases in cyclic or oscillatory models [215]. One then has a history of many cycles separated by bounces, whose duration depends on details of the model such as the potential. Here also, results have to be interpreted carefully since especially such long-term evolutions are sensitive to all possible quantum corrections, not just those included here. There can then be many brief cycles until eventually, if the potential is right, one obtains an inflationary phase, if the scalar has grown high enough. In this way, one can develop an idea of the history of our universe before the Big Bang. The possibility of using a bounce to describe the structure in the universe exists. So far this has only been described in models [200] using brane scenarios [219], in which the classical singularity has been assumed to be absent by yet-to-be-determined quantum effects. As it turns out, the explicit mechanism removing singularities in loop cosmology is not compatible with the assumptions made in those effective pictures. In particular, the scalar was supposed to turn around during the bounce, which is impossible in loop scenarios unless it encounters a range of positive potential during its evolution [98]. Then, however, an inflationary phase generally commences, as in [215, 244], which is then the relevant regime for structure formation. This shows how model building in loop cosmology can distinguish scenarios that are more likely to occur from quantum gravity effects.

Cyclic models can be argued to shift the initial moment of a universe in the infinite past, but they do not explain how the universe started. An attempt to explain this is the emergent universe model [160, 162], in which one starts close to a static solution. This is difficult to achieve classically, however, since the available fixed points of the equations of motion are not stable and thus a universe departs too rapidly. Loop cosmology, on the other hand, implies an additional fixed point of the effective equations, which is stable, and allows the universe to start in an initial phase of oscillations before an inflationary phase is entered [238, 61]. This presents a natural realization of the scenario in which the initial scale factor at a fixed point is automatically small so as to start the universe close to the Planck phase.

4.6.4 Stability

Cosmological equations displaying super-inflation or antifriction are often unstable in the sense that matter can propagate faster than light. This has been voiced as a potential danger for loop cosmology as well [139, 140]. An analysis requires inhomogeneous techniques, at least at an effective level, such as those described in Section 4.16. It has been shown that loop cosmology is free of this problem because the new behavior of the homogeneous mode of the metric and matter is not relevant for matter propagation [186]. The whole cosmological picture that follows from the effective equations is thus consistent.

4.7 Isotropy: Phenomenological higher curvature corrections

In addition to the behavior of effective densities, there is a further consequence of a discrete triad spectrum: Its conjugate c cannot exist as a self-adjoint operator because in that case it would generate arbitrary continuous translations in p. Instead, only exponentials of the form $\exp(i\delta c)$ can be quantized, where the parameter δ is related to the precise form of the discreteness of p. Corresponding operators in a triad representation of wave functions are finite differences rather than infinitesimal differentials, which also expresses the underlying discreteness. (This is analogous to quantum mechanics on a circle, although in loop quantum cosmology the discreteness is not based on a simple periodic identification but rather a more complicated compactification of the configuration space 5.2.)

Any classical expression when quantized has to be expressed in terms of functions of c, such as $\delta^{-1}\sin(\delta c)$, while common classical expressions, e.g., the Hamiltonian constraint (23), only depend on c directly or through powers. When $\delta^{-1}\sin(\delta c)$ occurs instead, the classical expression is reproduced at small values of c, i.e., small extrinsic curvature, but higher-order corrections are present [52, 36, 146, 299]. This provides a further discreteness effect in loop cosmology, which is part of the effective equations. The effect has several noteworthy properties:

- One should view the precise function $\sin(\delta c)$ as a simple placeholder for a perturbative expansion in powers of c, rather than a precise expansion with infinitely many terms. Even if one would use the function to represent a whole perturbation expansion, which is rarely allowed because there are additional quantum corrections of different forms dominating almost all terms in the series, it would still be a perturbative quantum correction. This distinguishes this type of correction from effective densities, which have a non-perturbative contribution involving inverse powers of the Planck length. Thus these two types of corrections appear on rather different footings.

- Seen as higher curvature corrections, higher power corrections in c cannot be complete because they do not provide higher derivative terms of a. They represent only one phenomenological effect, which originates from quantum geometry and provides some terms of higher curvature corrections. But, for a reliable evaluation of effective equations, they need to be combined with other corrections, whose origin we will describe in Section 6. This further distinguishes these higher power corrections from effective densities.

- The parameter δ can be scale dependent, i.e., a function of the triad $\delta(p)$. As p increases and the universe expands, the discreteness realized in a quantum state in general changes; see Section 3.7. Thus, δ must change with p to describe the precise discreteness realized at different volumes. More details are provided in Section 5.5 and 6.4.

4.8 Isotropy: Intuitive meaning of higher power corrections

Higher-power corrections represent an independent implication of the discreteness of quantum geometry. It is thus interesting to compare their possible effects with those of effective densities and to see if they support each other or act antagonistically. A basic observation indicates supportive behavior because higher-power corrections can also be associated with repulsive contributions to the gravitational force at small scales. The origin is not as intuitive as with effective densities because higher powers of c or $\dot{a}$ cannot be understood in analogy to classical mechanics, in which the emergence of new forces would be imminent.

Instead, one can understand the repulsive behavior directly as a consequence of the discreteness of quantum geometry. Rather than providing an infinite reservoir of a continuous spacetime medium, quantum geometry as a discrete structure has only finite storage space for energy. When energy densities become too high, e.g., near a classical singularity, they can no longer be supported by quantum geometry, while classical geometry easily allows an infinite increase of energy densities. Like a sponge, which when fully soaked repels further water, quantum spacetime reacts to high energy densities with repulsive forces. This expectation is also borne out by specific phenomenological and effective analysis of higher-power models.

4.9 Isotropy: Applications of higher-power corrections

A simple model, which has played several important roles in this context, illustrates the basic features of higher-power corrections very well. This model is isotropic, spatially flat and sourced by a free, massless scalar. It was first looked at in the context of loop quantum cosmology in [89, 181] from the point of view of difference equations and boundary proposals. More recently, it was realized that the absence of a scalar potential allows the explicit derivation of the physical inner product and detailed numerical calculations of physical states [26], as well as the derivation of exact effective equations [70]. The relation to effective equations will be discussed in Section 6.3. For now, we can observe that the boundedness of functions such as $\sin(\delta c)$, which can arise from the discreteness directly, implies a lower bound to the volume of such models. In the effective Friedmann equation,

$$\delta^{-2}\sin^2(\delta c)\sqrt{|p|} = \frac{8\pi G}{6}\frac{p_\phi^2}{|p|^{3/2}}, \tag{34}$$

the scalar momentum is constant due to the absence of a potential for the free scalar. Thus, $p^{-2} \propto \sin^2(\delta c) \leq 1$ shows that $|p|$ must be bounded away from zero; the scale factor bounces instead of reaching a classical singularity at $p = 0$. The precise bounce scale depends on the form of $\delta(p)$.

One can translate this into a phenomenological Friedmann equation involving the scale factor and its time derivative. The Hamiltonian equation of motion for p implies

$$\dot{p} = 2\delta^{-1}\sqrt{|p|}\sin(\delta c)\cos(\delta c)$$

and thus

$$\left(\frac{\dot{a}}{a}\right)^2 = 4\left(\frac{\dot{p}}{p}\right)^2 = \frac{8\pi G}{6}\frac{p_\phi^2}{|p|^{3/2}}\left(1 - \frac{8\pi G}{6}\frac{p_\phi^2}{|p|^{3/2}}p\delta^2\right) \tag{35}$$

when this is inserted into Equation (34). (The right-hand side depends on the energy density but not on p, for $\delta(p) \propto 1/|p|^{1/2}$, which is sometimes preferred [278].) The whole series of higher-power corrections thus implies only quadratic corrections for the energy density of a free scalar field [299, 278], which is usually easier and more insightful to analyze. One has to keep in mind, however, that this form of the equation is truly effective only in the absence of a scalar potential and of any deviations from isotropy. Otherwise there are further corrections, which prevent the equation from being brought into a simple quadratic energy-density form; see Section 6.

A similar form of effective equations can be used for a closed model, which, due to its classical recollapse now being combined with a quantum bounce, provides cyclic-universe models. These are no longer precise effective equations, but one can show that additional quantum corrections during the classical collapse phase are small. Thus, deviations from the phenomenological trajectory solving Equation (35) build up only slowly in time and require several cycles to become noticeable, as first analyzed and verified numerically in [28]. If one pretends that the same kind of quadratic corrections can be used for massive or self-interacting scalars, there is a rich phenomenology of cyclic universes, some of which has been analyzed in [281, 270, 271, 314, 307, 311, 287, 313, 151]. However, for such long evolution times it is crucial to consider all quantum effects, which for massive or self-interacting matter is not captured fully in the simple quadratic energy-density corrections.

Qualitatively, the appearance of bounces agrees with what we saw for effective densities, although the precise realization is different and occurs for different models. Moreover, if we bring together higher-power corrections, as well as effective densities, we see that, although individually they both have similar effects, together they can counteract each other. In the specific model considered here, using effective densities in the matter term and possibly the gravitational term results in an inequality of the form $f(p) \propto \sin^2(\delta c) \leq 1$ where $f(p)$ replaces the classical p^{-2} used above and has an upper bound. Thus, one cannot immediately conclude that p is bounded away from zero and rather has to analyze the precise numerical constants appearing in this relation. A conclusion about a bounce can then no longer be generic but will depend on initial conditions. This shows the importance of bringing all possible quantum corrections together in a consistent manner. It is also important to realize that, while Equation (34) is a precise effective equation for the dynamical behavior of a quantum state as described later, the inclusion of effective densities would imply further quantum corrections, which we have not described so far and which result from backreaction effects of a spreading state on its expectation values. These corrections would also have to be included for a complete analysis, which is still not finished.

Before all quantum corrections have been determined, one can often estimate their relative magnitudes. In the model considered here, this is possible when one uses the condition that a realistic universe must have a large matter content. Thus, p_ϕ must be large, which affects the constants in the above relations to the extent that the maximum of $f(p)$ will not be reached before $\sin(\delta c)$ reaches the value one. In this case there is thus a bounce independent of effective-density suppressions. Moreover, if one starts in a sufficiently semiclassical state at large volume, quantum backreaction effects will not change the evolution too much before the bounce is reached. Thus, higher power corrections are indeed dominant and can be used reliably. There are, however, several caveats: First, while higher-power corrections are relevant only briefly near the bounce, quantum backreaction is present at all times and can easily add up. Especially for systems with a different matter content such as a scalar potential, a systematic analysis has yet to be performed. Anisotropies and inhomogeneities can have a similar effect, but for inhomogeneities an additional complication arises: not all the matter is lumped into one single isotropic patch, but rather distributed over the discrete building blocks of a universe. Local matter contents are then much smaller than the total one, and the above argument for the dominance of higher-power corrections no longer applies. Finally, the magnitude of corrections in effective densities has been underestimated in most homogeneous studies so far because effects of lattice states were overlooked (see Appendix in [75]). They can thus become more important at small scales and possibly counteract a bounce, even if the geometry can safely be assumed to be nearly isotropic. Whether or not there is a bounce in such cases remains unknown at present.

4.10 Anisotropies

Anisotropic models provide a first generalization of isotropic ones to more realistic situations. They thus can be used to study the robustness of effects analyzed in isotropic situations and, at the same time, provide a large class of interesting applications. In particular, an analysis of the singularity issue is important since the classical approach to a singularity can be very different from the isotropic one. On the other hand, the anisotropic approach is deemed to be characteristic even for general inhomogeneous singularities, if the BKL scenario [38] is correct.

A general homogeneous but anisotropic metric is of the form

$$\mathrm{d}s^2 = -N(t)^2\,\mathrm{d}t^2 + \sum_{I,J=1}^{3} q_{IJ}(t)\omega^I \otimes \omega^J$$

with left-invariant 1-forms ω^I on space Σ, which, thanks to homogeneity, can be identified with the simply transitive symmetry group S as a manifold. The left-invariant 1-forms satisfy the

Maurer–Cartan relations

$$\mathrm{d}\omega^I = -\frac{1}{2} C^I_{JK} \omega^J \wedge \omega^K$$

with the structure constants C^I_{JK} of the symmetry group. In a matrix parameterization of the symmetry group, one can derive explicit expressions for ω^I from the Maurer–Cartan form $\omega^I T_I = \theta_{MC} = g^{-1}\mathrm{d}g$ with generators T_I of S.

The simplest case of a symmetry group is an Abelian one with $C^I_{JK} = 0$, corresponding to the Bianchi I model. In this case, S is given by $\mathbb{R}^3$ or a torus, and left-invariant 1-forms are simply $\omega^I = \mathrm{d}x^I$ in Cartesian coordinates. Other groups must be restricted to class A models in this context, satisfying $C^I_{JI} = 0$ since otherwise there is no standard Hamiltonian formulation [220]. The structure constants can then be parameterized as $C^I_{JK} = \epsilon^I_{JK} n^{(I)}$.

A common simplification is to assume the metric to be diagonal at all times, which corresponds to a reduction technically similar to a symmetry reduction. This amounts to $q_{IJ} = a^2_{(I)}\delta_{IJ}$ as well as $K_{IJ} = K_{(I)}\delta_{IJ}$ for the extrinsic curvature with $K_I = \dot{a}_I$. Depending on the structure constants, there is also non-zero intrinsic curvature quantified by the spin connection components

$$\Gamma_I = \frac{1}{2}\left(\frac{a_J}{a_K} n^J + \frac{a_K}{a_J} n^K - \frac{a_I^2}{a_J a_K} n^I\right) \quad \text{for} \quad \epsilon_{IJK} = 1\,. \tag{36}$$

This influences the evolution as follows from the Hamiltonian constraint

$$-\frac{1}{8\pi G}\big(a_1\dot{a}_2\dot{a}_3 + a_2\dot{a}_1\dot{a}_3 + a_3\dot{a}_1\dot{a}_2 - (\Gamma_2\Gamma_3 - n^1\Gamma_1)a_1 - (\Gamma_1\Gamma_3 - n^2\Gamma_2)a_2 \\ - (\Gamma_1\Gamma_2 - n^3\Gamma_3)a_3\big) + H_{\mathrm{matter}}(a_I) = 0\,. \tag{37}$$

In the vacuum Bianchi I case the resulting equations are easy to solve by $a_I \propto t^{\alpha_I}$ with $\sum_I \alpha_I = \sum_I \alpha_I^2 = 1$ [198]. The volume $a_1a_2a_3 \propto t$ vanishes for $t = 0$ where the classical singularity appears. Since one of the exponents α_I must be negative, however, only two of the a_I vanish at the classical singularity, while the third one diverges. This already demonstrates how different the behavior can be from the isotropic model and that anisotropic models provide a crucial test of any mechanism for singularity resolution.

4.11 Anisotropy: Connection variables

A densitized triad corresponding to a diagonal homogeneous metric has real components p^I with $|p^I| = a_J a_K$ if $\epsilon_{IJK} = 1$ [56]. Connection components are $c_I = \Gamma_I + \gamma K_I = \Gamma_I + \gamma\dot{a}_I$ and are conjugate to the p_I, $\{c_I, p^J\} = 8\pi\gamma G\delta^J_I$. In terms of triad variables we now have spin connection components

$$\Gamma_I = \frac{1}{2}\left(\frac{p^K}{p^J} n^J + \frac{p^J}{p^K} n^K - \frac{p^J p^K}{(p^I)^2} n^I\right) \tag{38}$$

and the Hamiltonian constraint (in the absence of matter)

$$H = \frac{1}{8\pi G}\Bigg\{\left[(c_2\Gamma_3 + c_3\Gamma_2 - \Gamma_2\Gamma_3)(1+\gamma^{-2}) - n^1c_1 - \gamma^{-2}c_2c_3\right]\sqrt{\left|\frac{p^2p^3}{p^1}\right|} \\ + \left[(c_1\Gamma_3 + c_3\Gamma_1 - \Gamma_1\Gamma_3)(1+\gamma^{-2}) - n^2c_2 - \gamma^{-2}c_1c_3\right]\sqrt{\left|\frac{p^1p^3}{p^2}\right|} \\ + \left[(c_1\Gamma_2 + c_2\Gamma_1 - \Gamma_1\Gamma_2)(1+\gamma^{-2}) - n^3c_3 - \gamma^{-2}c_1c_2\right]\sqrt{\left|\frac{p^1p^2}{p^3}\right|}\Bigg\}\,. \tag{39}$$

Unlike in isotropic models, we now have inverse powers of p^I, even in the vacuum case, through the spin connection, unless we are in the Bianchi I model. This is a consequence of the fact that not just extrinsic curvature, which in the isotropic case is related to the matter Hamiltonian through the Friedmann equation, leads to divergences but also intrinsic curvature. These divergences are cut off by quantum geometry effects as before, such that the dynamical behavior also changes. This can again be dealt with by phenomenological equations where inverse powers of triad components are replaced by bounded functions [82]. However, even with those corrections, expressions for curvature are not necessarily bounded unlike in the isotropic case. This comes from the presence of different classical scales, a_I, such that more complicated expressions as in Γ_I are possible, while in the isotropic model there is only one scale and curvature can only be an inverse power of p, which is then regulated by effective expressions like $d(p)$.

4.12 Anisotropy: Applications

4.12.1 Isotropization

Matter fields are not the only contributions to the Hamiltonian in cosmology. The effect of anisotropies can also be included in an isotropic model in this way. The late time behavior of this contribution can be shown to behave as a^{-6} in the shear energy density [228], which falls off faster than any other matter component. Thus, toward later times the universe becomes more and more isotropic.

In backward evolution, on the other hand, this means that the shear term diverges most strongly, which suggests that this term should be most relevant for the singularity issue. Even if matter densities are cut off as discussed before, the presence of bounces would depend on the fate of the anisotropy term. This simple reasoning is not true, however, since the behavior of shear is only effective and uses assumptions about the behavior of matter. Thus, it cannot simply be extrapolated to early times. Anisotropies are independent degrees of freedom which affect the evolution of the scale factor. Only in certain regimes can this contribution be modeled simply by a function of the scale factor alone; in general, one has to use the coupled system of equations for the scale factor, anisotropies and possible matter fields.

4.12.2 Bianchi IX

Corrections to classical behavior are most drastic in the Bianchi IX model with symmetry group $S \cong \mathrm{SU}(2)$ such that $n^I = 1$. The classical evolution can be described by a 3-dimensional mechanics system with a potential obtained from Equation (37) such that the kinetic term is quadratic in derivatives of a_I with respect to a time coordinate τ defined by $\mathrm{d}t = a_1a_2a_3\mathrm{d}\tau$. This potential

$$\begin{aligned} W(p^I) &= (\Gamma_2\Gamma_3 - n^1\Gamma_1)p^2p^3 + (\Gamma_1\Gamma_3 - n^2\Gamma_2)p^1p^3 + (\Gamma_1\Gamma_2 - n^3\Gamma_3)p^1p^2 \\ &= \frac{1}{4}\left(\left(\frac{p^2p^3}{p^1}\right)^2 + \left(\frac{p^1p^3}{p^2}\right)^2 + \left(\frac{p^1p^2}{p^3}\right)^2 - 2(p^1)^2 - 2(p^2)^2 - 2(p^3)^2\right) \end{aligned} \tag{40}$$

diverges at small p^I, in particular (in a direction-dependent manner) at the classical singularity where all $p^I = 0$. Figure 4 illustrates the walls of the potential, which with decreasing volume push the universe toward the classical singularity.

As before in isotropic models, phenomenological equations in which the behavior of eigenvalues of the spin connection components is used, do not have this divergent potential. Instead, if two p^I are held fixed and the third approaches zero, the effective potential is cut off and goes back to zero at small values, which changes the approach to the classical singularity. Yet, the effective potential is unbounded if one p^I diverges while another goes to zero and the situation is qualitatively different from the isotropic case. Since the effective potential corresponds to spatial intrinsic curvature,

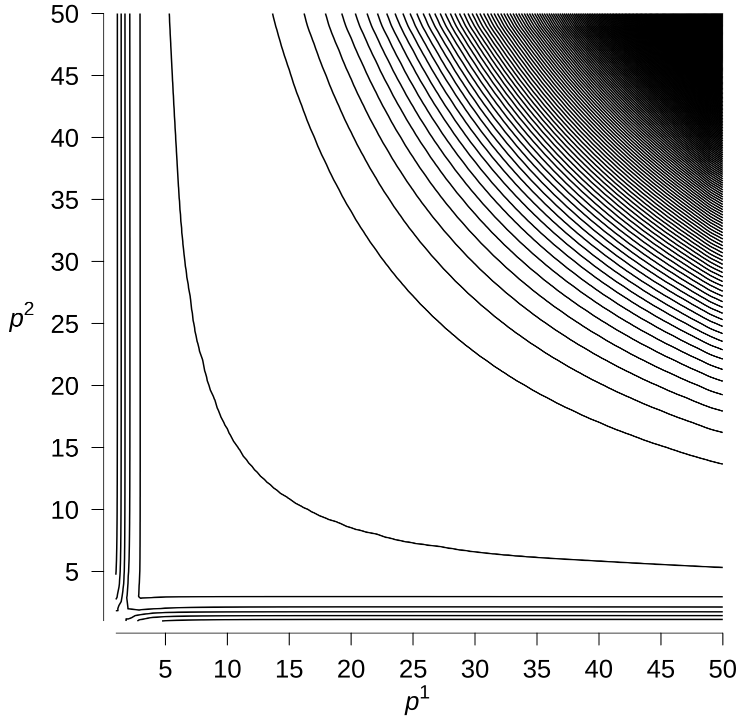

Figure 4: Still from a movie showing An illustration of the Bianchi IX potential (40) and the movement of its walls, rising toward zero p^1 and p^2 and along the diagonal direction, toward the classical singularity with decreasing volume $V = \sqrt{|p^1 p^2 p^3|}$. The contours are plotted for the function $W(p^1, p^2, V^2/(p^1 p^2))$. (To watch the movie, please go to the online version of this review article at `http://www.livingreviews.org/lrr-2008-4`.)

curvature is *not bounded* in anisotropic effective models. However, this is a statement only about (kinematical) curvature expressions on minisuperspace, and the more relevant question is what happens to curvature along dynamical trajectories obtained by solving equations of motion. This demonstrates that dynamical equations must always be considered to draw conclusions for the singularity issue.

The approach to the classical singularity is best analyzed in Misner variables [229] consisting of the scale factor $\Omega := -\frac{1}{3}\log V$ and two anisotropy parameters $\beta_\pm$ defined such that

$$a_1 = e^{-\Omega+\beta_+ + \sqrt{3}\beta_-}\,, \qquad a_2 = e^{-\Omega+\beta_+ - \sqrt{3}\beta_-}\,, \qquad a_3 = e^{-\Omega-2\beta_+}\,.$$

The classical potential then takes the form

$$W(\Omega,\beta_\pm) = \frac{1}{2}e^{-4\Omega}\left(e^{-8\beta_+} - 4e^{-2\beta_+}\cosh(2\sqrt{3}\beta_-) + 2e^{4\beta_+}(\cosh(4\sqrt{3}\beta_-) - 1)\right)\,,$$

which at fixed Ω has three exponential walls rising from the isotropy point $\beta_\pm = 0$ and enclosing a triangular region (see Figure 5).

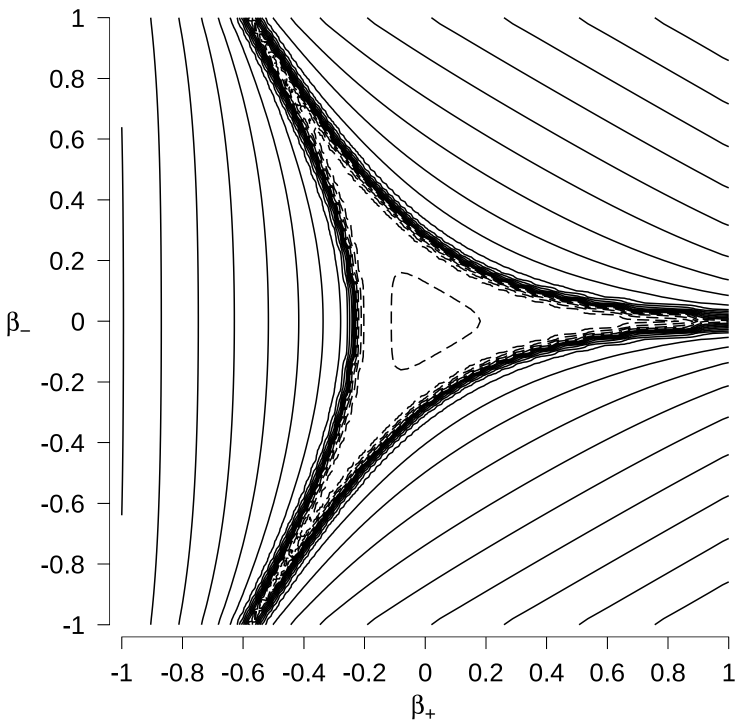

Figure 5: Still from a movie showing An illustration of the Bianchi IX potential in the anisotropy plane and its exponentially rising walls. Positive values of the potential are drawn logarithmically with solid contour lines and negative values with dashed contour lines. (To watch the movie, please go to the online version of this review article at `http://www.livingreviews.org/lrr-2008-4`.)

A cross section of a wall can be obtained by taking $\beta_- = 0$ and $\beta_+ < 0$, in which case the potential becomes $W(\Omega,\beta_+,0) \approx \frac{1}{2}e^{-4\Omega-8\beta_+}$. One obtains the picture of a point moving almost freely until it is reflected at a wall. In between reflections, the behavior is approximately given by the Kasner solution described previously. This behavior, with infinitely many reflections before the classical singularity is reached, can be shown to be chaotic [39], which suggests a complicated approach to classical singularities in general.

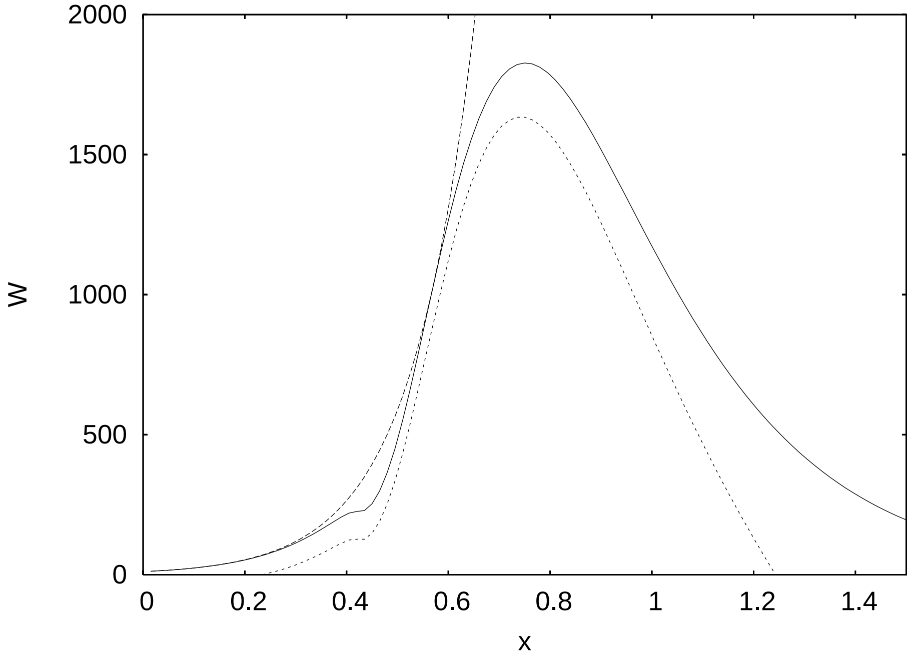

Figure 6: Approximate effective wall of finite height [80] as a function of $x = -\beta_+$, compared to the classical exponential wall (upper dashed curve). Also shown is the exact wall $W(p^1, p^1, (V/p^1)^2)$ (lower dashed curve), which for x smaller than the peak value coincides well with the approximation up to a small, nearly constant shift.

With the effective-density term, however, the potential for fixed Ω does not diverge and the walls, as shown in Figure 6, break down at a small but non-zero volume [80]. The effective potential is illustrated in Figure 7 as a function of densitized triad components and as a function on the anisotropy plane in Figure 8. In this scenario, there are only a finite number of reflections, which do not lead to chaotic behavior but instead result in asymptotic Kasner behavior [81].

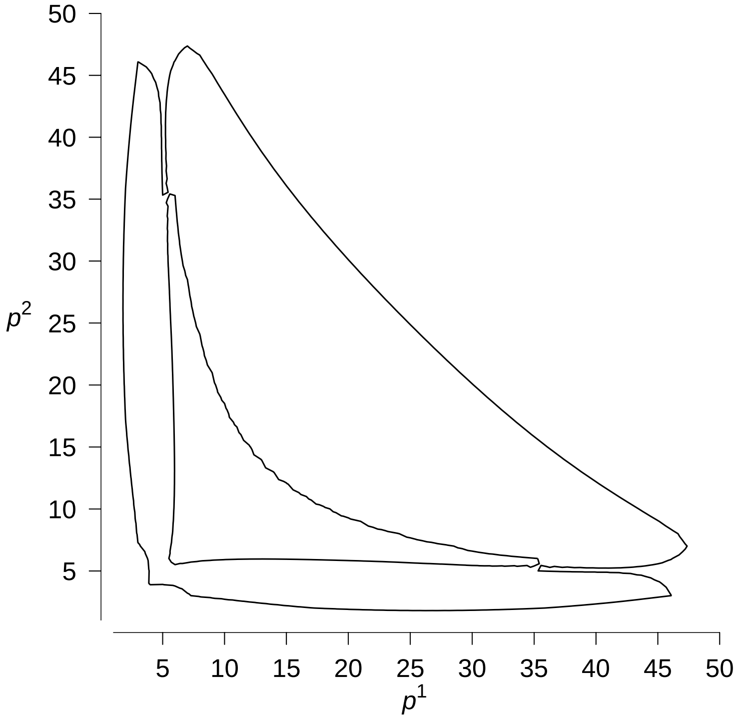

Figure 7: Still from a movie showing An illustration of the effective Bianchi IX potential and the movement and breakdown of its walls. The contours are plotted as in Figure 4. (To watch the movie, please go to the online version of this review article at `http://www.livingreviews.org/lrr-2008-4`.)

Comparing Figure 5 with Figure 8 shows that at their centers they are very close to each other, while strong deviations occur for large anisotropies. This demonstrates that most of the classical evolution, which happens almost entirely in the inner triangular region, is not strongly modified by the effective potential. Quantum effects are important only when anisotropies become too large, for instance when the system moves deep into one of the three valleys, or the total volume becomes small. In those regimes the quantum evolution will take over and describe the further behavior of the system.

4.12.3 Isotropic curvature suppression

If we use the potential for time coordinate t rather than τ, it is replaced by $W/(p^1p^2p^3)$, which in the isotropic reduction $p^1 = p^2 = p^3 = \frac{1}{4}a^2$ gives the curvature term ka^{-2}. Although the anisotropic effective curvature potential is not bounded, it is, unlike the classical curvature, bounded from above at any fixed volume. Moreover, it is bounded along the isotropy line and decays when a approaches zero. Thus, there is a suppression of the divergence in ka^{-2} when the closed isotropic model is viewed as embedded in a Bianchi IX model. Similar to matter Hamiltonians, intrinsic curvature then approaches zero at zero scale factor.

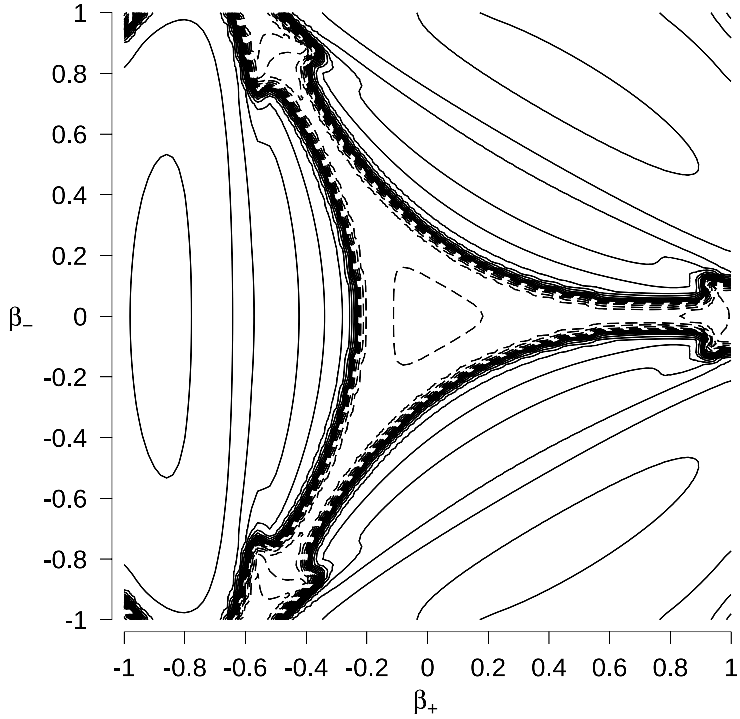

Figure 8: Still from a movie showing An illustration of the effective Bianchi IX potential in the anisotropy plane and its walls of finite height, which disappear at finite volume. Positive values of the potential are drawn logarithmically with solid contour lines and negative values with dashed contour lines. (To watch the movie, please go to the online version of this review article at `http://www.livingreviews.org/lrr-2008-4`.)

This is a further illustration of the special nature of isotropic models compared to anisotropic ones. In the classical reduction, the p^I in the anisotropic spin connection cancel such that the spin connection is a constant and no special steps are needed for its quantization. By viewing isotropic models within anisotropic ones, one can consistently realize the model and see a suppression of intrinsic curvature terms. Anisotropic models, on the other hand, do not have, and do not need, complete suppression since curvature functions can still be unbounded.

4.13 Anisotropy: Phenomenological higher curvature

As in isotropic models, the discreteness of geometry also provides corrections of higher powers of extrinsic curvature components, and these can take different forms depending on how the discreteness of an underlying state changes during evolution. Due to the larger number of degrees of freedom, there are now more options for the behavior and a larger variety of potential phenomena. Viable classes of discretization effects are, however, rather strongly restricted by the requirement of showing the correct semiclassical behavior in the right regimes [75, 128]. Thus, even without developing a precise relation between a full Hamiltonian constraint and the effects it implies for the refinement in a model, one can self-consistently test symmetric models, although only initial steps [127, 126, 125] toward a comprehensive analysis have been undertaken.

Anisotropic solutions as analogs for Kasner solutions in the presence of higher powers of extrinsic curvature have first been studied in [142], although without considering refinements of the discreteness scale. These solutions have already shown that anisotropic models also exhibit bounces when such corrections are included phenomenologically, i.e., disregarding quantum backreaction. The issue has been revisited in [128, 42] for models including refinement (and a free, massless scalar as internal time) with the same qualitative conclusions. Similar calculations have been applied to Kantowski–Sachs models, which classically provide the Schwarzschild interior metric, without refinement in [231, 232] and with two different versions of refinement in [42]. They can thus be used to obtain indications for the behavior of quantum black holes, at least in the vacuum case. Then, however, one cannot use the arguments, which in isotropic cosmological models allowed one to conclude that higher-power corrections are dominant given a large matter content. Correspondingly, bounces of the higher-power phenomenological equations happen at much smaller scales than in massive isotropic models. They are thus less reliable because other corrections can become strong in those regimes.

4.14 Anisotropy: Implications for inhomogeneities

Even without implementing inhomogeneous models the previous discussion allows some tentative conclusions as to the structure of general singularities. This is based on the BKL picture [38], whose basic idea is to study Einstein's field equations close to a singularity. One can then argue that spatial derivatives become subdominant compared to time-like derivatives such that the approach should locally be described by homogeneous models, in particular the Bianchi IX model, since it has the most freedom in its general solution.

Since spatial derivatives are present, though, they lead to small corrections and couple the geometries in different spatial points. One can visualize this by starting with an initial slice, which is approximated by a collection of homogeneous patches. For some time, each patch evolves independently of the others, but this is not precisely true since coupling effects have been ignored. Moreover, each patch geometry evolves in a chaotic manner, which means that two initially nearby geometries depart rapidly from each other. The approximation can thus be maintained only if the patches are subdivided during the evolution, which goes on without limits in the approach to the singularity. There is, thus, more and more inhomogeneous structure being generated on arbitrarily small scales, which leads to a complicated picture of a general singularity.

This picture can be used to describe the behavior of the Bianchi IX model with effective density corrections (higher powers of the connection have not yet been included). Here, the patches do not evolve chaotically, even though at larger volume they follow the classical behavior. The subdivision thus has to also be done for the initial effective evolution. At some point, however, when reflections on the potential walls stop, the evolution simplifies and subdivisions are no longer necessary. There is thus a lower bound to the scale of structure, whose precise value depends on the initial geometries. Nevertheless, from the scale at which the potential walls break down, one can show that structure formation stops at the latest when the discreteness scale of quantum geometry is reached [80]. This can be seen as a consistency test of the theory, since structure below the discreteness could not be supported by quantum geometry.

We have thus a glimpse of the inhomogeneous situation with a complicated but consistent approach to a general classical singularity. The methods involved, however, are not very robust, since the BKL scenario, which despite some progress at analytical and numerical levels [249, 169] is even classically still at the level of a conjecture for the general case [39, 249], would need to be available as an approximation to quantum geometry. For more reliable results the methods need to be refined to take into account inhomogeneities properly.

Applications of the BKL picture are, however, in trouble, if bounces are a generic phenomenon of effective equations. The BKL scenario is an asymptotic statement about the behavior of solutions near a curvature singularity. When solutions bounce in the presence of quantum corrections, they may never reach a regime where asymptotic statements of this form apply, thus preventing the use of the BKL picture (although alternative pictures in the same spirit may become available). To be precise, some solutions may be tuned such that they do not bounce before an asymptotic regime is reached, where one could then use the BKL decoupling of different patches together with bounces in anisotropic models to conclude that even corresponding inhomogeneous solutions are non-singular. Since this requires special initial conditions to be able to enter an asymptotic regime before bounces occur, such a procedure could not provide general singularity removal. (See also [71] for a more detailed discussion of general singularities.)

4.15 Inhomogeneities

Allowing for inhomogeneities inevitably means taking a big step from finitely many degrees of freedom to infinitely many ones. There is no straightforward way to cut down the number of degrees of freedom to finitely many ones while being more general than in the homogeneous context. One possibility would be to introduce a small-scale cutoff such that only finitely many wave modes arise, e.g., through a lattice, as is indeed done in some coherent state constructions [269]. This is in fact expected to happen in a discrete framework such as quantum geometry, but would, at this stage of defining a model, simply be introduced by hand.

For the analysis of inhomogeneous situations there are several different approximation schemes:

- Use only isotropic quantum geometry and in particular its effective description, but couple it to inhomogeneous matter fields. Some problems to this approach include backreaction effects that are ignored (which is also the case in most classical treatments) and that there is no direct way to check modifications used, in particular for gradient terms of the matter Hamiltonian. So far, this approach has led to a few indications of possible effects.

- Start with the full constraint operator, write it as the homogeneous one plus correction terms from inhomogeneities, and derive effective classical equations. This approach is more ambitious since contact to the full theory is realized. Several correction terms for different metric modes in linearized perturbation theory have been computed [84, 90, 91, 92], although complete effective equations are not yet available. These equations already show the potential not only for phenomenological applications in cosmology but also to test fundamental issues such as the anomaly problem and covariance; see Section 6.5.4.

- There are inhomogeneous symmetric models, such as the spherically-symmetric one or Einstein–Rosen waves, which have infinitely many kinematical degrees of freedom but can be treated explicitly. Contact to the full theory is present here as well, through the symmetry-reduction procedure of Section 7. This procedure itself can be tested by studying those models with a complexity between homogeneous ones and the full theory, but results can also be used for physical applications involving inhomogeneities. Many issues that are of importance in the full theory, such as the anomaly problem, also arise here and can thus be studied more explicitly.

4.16 Inhomogeneous matter with isotropic quantum geometry

Inhomogeneous matter fields cannot be introduced directly to isotropic quantum geometry since, after the symmetry reduction, there is no space manifold left for the fields to live on. There are then two different routes to proceed: one can simply take the classical field Hamiltonian and introduce phenomenological modifications modeled on what happens to the isotropic Hamiltonian, or perform a mode decomposition of the matter fields and just work with the space-independent amplitudes. The latter is possible since the homogeneous geometry provides a background for the mode decomposition to be defined.

The basic question then, for the example of a scalar field, is how to replace the metric coefficient $E^a_i E^b_i/\sqrt{|\det E|}$ in the gradient term of Equation (12). For the other terms, one can simply use the isotropic modification, which is taken directly from the quantization. For the gradient term, however, one does not have a quantum expression in this context and a modification can only be guessed. The problem arises because the inhomogeneous term involves inverse powers of E, while in the isotropic context the coefficient just reduces to $\sqrt{|p|}$, which would not receive corrections at all. There is thus no obvious and unique way to find a suitable replacement.

A possible route would be to read off the corrections from the full quantum Hamiltonian, or at least from an inhomogeneous model, which requires a better knowledge of the reduction procedure. Alternatively, one can take a more phenomenological point of view and study the effects of different possible replacements. If the robustness of these effects to changes in the replacements is known, one can get a good picture of possible implications. So far, only initial steps have been taken (see [182] for scalar modes and [226] for tensor modes) and there is no complete program in this direction.

Another approximation of the inhomogeneous situation has been developed in [100] by patching isotropic quantum geometries together to support an inhomogeneous matter field. This can be used to study modified dispersion relations to the extent that the result agrees with preliminary calculations performed in the full theory [168, 3, 4, 267, 268] even at a quantitative level. There is thus further evidence that symmetric models and their approximations can provide reliable insights into the full theory.

4.17 Inhomogeneity: Perturbations

With a symmetric background, a mode decomposition is not only possible for matter fields but also for geometry. The homogeneous modes can then be quantized as before, while higher modes are coupled as perturbations implementing inhomogeneities [175]. As with matter Hamiltonians before, one can then also deal with the gravitational part of the Hamiltonian constraint. In particular, there are terms with inverse powers of the homogeneous fields, which receive corrections upon quantization. As with gradient terms in matter Hamiltonians, there are several options for those corrections, which can be restricted by relating them to the full Hamiltonian but also by requiring anomaly freedom at the effective level.

This requires introducing the mode decomposition, analogous to symmetry conditions, at the quantum level and splitting the full constraint into the homogeneous one plus correction terms. One can perform a quantum mode decomposition by specializing the full theory to regular lattices defined using the background model as the embedding space. This can be used to simplify basic operators of the full theory in a way similar to symmetric models, although no restriction of classical degrees of freedom happens at this level. For the simplest modes in certain gauges the Hamiltonian constraint operator becomes computable explicitly [86], which is the first step in the derivation of effective constraints. From the Hamiltonian constraint one obtains an effective expression in terms of discrete variables associated with the lattice state, and in a subsequent continuum approximation one arrives at equations of the classical form but including quantum corrections. There is thus no continuum limit at the quantum level, which avoids difficulties similar to those faced by a Wheeler–DeWitt quantization of inhomogeneous models.

Effective equations thus result in two steps, including the continuum approximation (see also Section 6.4). The result contains corrections of the same types as in homogeneous models: effective densities, higher powers of extrinsic curvature and quantum backreaction effects. In contrast to homogeneous models, however, the relative dominance of these corrections is different. Corrections now come from individual lattice sites and qualitatively agree with the homogeneous corrections, but are evaluated in local lattice variables rather than global ones such as the total volume. Thus, the arguments of effective densities as well as higher power functions such as $\sin(\delta c)$ are now much smaller than they would be in an exactly homogeneous model. Both types of corrections are affected differently by decreasing their arguments: effective-density corrections increase for smaller arguments while higher-power corrections decrease. This makes effective-density corrections much more relevant in inhomogeneous situations than they appear in homogeneous ones [66].

4.18 Inhomogeneous models

The full theory is complicated at several different levels of both its conceptual and technical nature. For instance, one has to deal with infinitely many degrees of freedom, most operators have complicated actions, and interpreting solutions to all constraints in a geometrical manner can be difficult. Most of these complications are avoided in homogeneous models, in particular when phenomenological equations of different types or precise effective equations are employed. These equations use approximations of expectation values of quantum geometrical operators, which need to be known rather explicitly. The question then arises of whether one can still work at this level while relaxing the symmetry conditions and bringing in more complications of the full theory.

Explicit calculations at a level similar to homogeneous models, at least for matrix elements of individual operators, are possible in inhomogeneous models, too. In particular, the spherically-symmetric model and cylindrically-symmetric Einstein–Rosen waves are of this class, in which the symmetry or other conditions are strong enough to result in a simple volume operator. In the spherically-symmetric model, this simplification comes from the remaining isotropy subgroup isomorphic to U(1) in generic points, while the Einstein–Rosen model is simplified by polarization conditions that play a role analogous to the diagonalization of homogeneous models. With these models one obtains access to applications for black holes and gravitational waves, but also to inhomogeneities in cosmology. Nevertheless, in spite of significant calculational simplifications, several fundamental issues remain to be resolved, such as a satisfactory quantum treatment of the constraint algebras arising in gravity.

In spherical coordinates x, ϑ, φ a spherically-symmetric spatial metric takes the form

$$\mathrm{d}s^2 = q_{xx}(x,t)\,\mathrm{d}x^2 + q_{\varphi\varphi}(x,t)\,\mathrm{d}\Omega^2$$

with $\mathrm{d}\Omega^2 = \mathrm{d}\vartheta^2 + \sin^2\vartheta\,\mathrm{d}\varphi^2$. This is related to densitized triad components by [294, 199]

$$|E^x| = q_{\varphi\varphi}\,, \qquad (E^\varphi)^2 = q_{xx}q_{\varphi\varphi},$$

which are conjugate to the other basic variables given by the Ashtekar connection component A_x and the extrinsic curvature component K_φ:

$$\{A_x(x), E^x(y)\} = 8\pi G\gamma\delta(x,y)\,, \qquad \{\gamma K_\varphi(x), E^\varphi(y)\} = 16\pi G\gamma\delta(x,y)\,.$$

Note that we use the Ashtekar connection for the inhomogeneous direction x but extrinsic curvature for the homogeneous direction along symmetry orbits [109]. Connection and extrinsic curvature components for the φ-direction are related by $A_\varphi^2 = \Gamma_\varphi^2 + \gamma^2 K_\varphi^2$ with the spin connection component

$$\Gamma_\varphi = -\frac{E^{x\prime}}{2E^\varphi}\,. \tag{41}$$

Unlike in the full theory or homogeneous models, A_φ is not conjugate to a triad component but to [60]

$$P^\varphi = \sqrt{4(E^\varphi)^2 - A_\varphi^{-2}(P^\beta)^2}$$

with the momentum P^β conjugate to a U(1)-gauge angle β. This is a rather complicated function of both triad and connection variables such that the volume $V = 4\pi\int\sqrt{|E^x|}E^\varphi\mathrm{d}x$ would have a complicated quantization. It would still be possible to compute the full volume spectrum, but with the disadvantage that volume eigenstates would not be given by triad eigenstates such that computations of many operators would be complicated [107]. This can be avoided by using extrinsic curvature, which is conjugate to the triad component [109]. Moreover, it is also in accordance with a general scheme to construct Hamiltonian constraint operators for the full theory as well as symmetric models [292, 50, 68].

The constraint operator in spherical symmetry is given by

$$H[N] = -(2G)^{-1}\int_B \mathrm{d}x N(x)|E^x|^{-1/2}\left((K_\varphi^2 E^\varphi + 2K_\varphi K_x E^x) + (1-\Gamma_\varphi^2)E^\varphi + 2\Gamma_\varphi' E^x\right) \tag{42}$$

accompanied by the diffeomorphism constraint

$$D[N^x] = (2G)^{-1}\int_B N^x(x)(2E^\varphi K_\varphi' - K_x E^{x\prime})\,. \tag{43}$$

We have expressed this in terms of K_x for simplicity, keeping in mind that we will later use the connection component A_x as the basic variable for quantization.

Since the Hamiltonian constraint contains the spin connection component Γ_φ given by (41), which contains inverse powers of densitized triad components, one can expect effective classical equations with corrections similar to the Bianchi IX model. Moreover, an inverse of E^x occurs in (42). However, the situation is now much more complicated, since we have a system bound by many constraints with non-Abelian algebra. Simply replacing the inverse of E^x or E^φ with a bounded function as before will change the constraint algebra and thus most likely lead to anomalies. In addition, higher powers of connection components or extrinsic curvature arise from holonomies and further correction terms from quantum backreaction. This issue has the potential to shed light on many questions related to the anomaly issue, as done for inverse corrections in [102]. It is one of the cases where models that lie between homogeneous ones, where the anomaly problem trivializes, and the full theory are most helpful.

4.19 Inhomogeneity: Results

There are some results obtained for inhomogeneous systems. We have already discussed glimpses from the BKL picture, which used loop results only for anisotropic models. Methods described in this section have led to some preliminary insights into possible cosmological scenarios.

4.19.1 Matter gradient terms and small-a effects

When an inhomogeneous matter Hamiltonian is available it is possible to study its implications on the cosmic microwave background with standard techniques. With quantum-corrected densities there are then different regimes, since the part of the inflationary era responsible for the formation of currently visible structure can be in the small-a or large-a region of the effective density.

The small-a regime, below the peak of effective densities, has more dramatic effects since inflation can here be provided by quantum geometry effects alone and the matter behavior changes to be anti-frictional [53, 111]. Mode evolution in this regime has been investigated for a particular choice of gradient term and using a power-law approximation for the effective density at small a, with the result that there are characteristic signatures [187]. As in standard inflation models, the spectrum is nearly scale invariant, but its spectral index is slightly larger than one (blue tilt) as compared to slightly smaller than one (red tilt) for single-field inflaton models. Since small scale factors at early stages of inflation generate structure which today appears on the largest scales, this implies that low multipoles of the power spectrum should have a blue tilt. The running of the spectral index in this regime can also be computed but depends only weakly on ambiguity parameters.

The main parameter then is the duration of loop inflation. In the simplest scenario, one can assume only one inflationary phase, which would require huge values for the ambiguity parameter j. This is unnatural and would likely imply that the spectrum is blue on almost all scales, which is in conflict with present observations. Thus, not only conceptual arguments but also cosmological observations point to smaller values for j, which is quite remarkable. On the other hand, while one cannot achieve a large ratio of scale factors during a single phase of super-inflation with small j, the ratio of the Hubble parameter multiplied by the scale factor increases more strongly. This is in fact the number relevant for structure formation, and so even smaller j may provide the right expansion for a viable power spectrum [134].

However, cosmological perturbation theory in this regime of non-perturbative corrections is more subtle than on larger scales [86], and so a precise form of the power spectrum is not yet available. Several analyses have been performed based on the classical perturbation theory but with super-inflationary quantum corrections for the isotropic background [237, 121, 134], showing that scale-invariant spectra can be obtained from certain classes of matter potentials driving the background in a suitable way; see also [226, 227] for a preliminary analysis of tensor modes on a super-inflationary background.

In order to have sufficient inflation to make the universe big enough, one then needs additional stages provided by the behavior of matter fields. One still does not need an inflaton since now the details of the expansion after the structure generating phase are less important. Any matter field being driven away from its potential minimum during loop inflation and rolling down its potential thereafter suffices. Depending on the complexity of the model there can be several such phases.

4.19.2 Matter gradient terms and large-a effects

At larger scale factors above the peak of effective densities there are only perturbative corrections from loop effects. This has been investigated with the aim of finding trans-Planckian corrections to the microwave background, here also with a particular gradient term [182].

A common problem of both analyses is that the robustness of the observed effects has not yet been studied. This is particularly a pressing problem since one modification of the gradient term has been chosen without further motivation. Moreover, the modifications of several examples were different. Without a more direct derivation of the corrections from inhomogeneous models or the full theory, one can only rely on a robustness analysis to show that the effects can be trusted. In addition, reliable conclusions are only possible if corrections in matter as well as gravitational terms of the Hamiltonian are taken into account; for the latter see Section 4.19.5.

4.19.3 Non-inflationary structure formation

Given a modification of the gradient term, one obtains effective equations for the matter field, which for a scalar results in a corrected Klein–Gordon equation. After a mode decomposition, one can then easily see that all the modes behave differently at small scales with the classical friction replaced by anti-friction as in Section 4.5. Thus, not only the average value of the field is driven away from its potential minimum but also higher modes are being excited. The coupled dynamics of all the modes thus provides a scenario for structure formation, which does not rely on inflation but on the anti-friction effect of loop cosmology.

Even though all modes experience this effect, they do not all see it in the same way. The gradient term implies an additive contribution to the potential proportional to k^2 for a mode of wave number k, which also depends on the metric in a way determined by the gradient term corrections. For larger scales, the additional term is not essential and their amplitudes will be pushed to similar magnitudes, suggesting scale invariance for them. The potential relevant for higher modes, however, becomes steeper and steeper such that they are less excited by anti-friction and retain a small initial amplitude. In this way, the structure formation scenario provides a dynamical mechanism for a small-scale cutoff, possibly realizing older expectations [246, 247].

In independent scenarios, phenomenological effects from loop cosmology have been seen to increase the viability of mechanisms to generate scale-invariant perturbations, such as in combination with thermal fluctuations [221].

4.19.4 Stability

As already noted, inhomogeneous matter Hamiltonians can be used to study the stability of cosmological equations in the sense that matter does not propagate faster than light. The behavior of homogeneous modes has led to the suspicion that loop cosmology is not stable [139, 140] since other cosmological models displaying super-inflation have this problem. A detailed analysis of the loop equations, however, shows that the equations as they arise from loop cosmology are automatically stable. While the homogeneous modes display super-inflationary and anti-frictional behavior, they are not relevant for matter propagation. Modes relevant for propagation, on the other hand, are corrected differently in such a manner that the total behavior is stable [186]. Most importantly, this is an example in which an inhomogeneous matter Hamiltonian with its corrections must be used and the qualitative result of stability can be shown to be robust under possible changes of the effective term. This shows that reliable conclusions can be drawn for important issues without a precise definition of the effective inhomogeneous behavior. Consistency has been confirmed for tensor modes based on a systematic analysis of anomaly cancellation in effective constraints [91].

4.19.5 Cosmological perturbation theory

For linear metric and matter perturbations the complete set of cosmological perturbation equations is available from a systematic analysis of scalar, vector and tensor modes [84, 92, 90, 91]. The main focus of those papers is on effective-density corrections both in the gravitational and matter terms. These equations have been formulated for gauge invariant perturbations (whose form also changes for quantum-corrected constraints) and thus provide physical results. By the very fact that such equations exist with non-trivial quantum corrections it has also been proven that loop quantum gravity can provide a consistent deformation of general relativity at least in linear regimes. Quantum corrections do allow anomaly-free effective constraints, which can then be written in a gauge-invariant form. The study of higher-power corrections has provided several consistency tests and restricted the class of allowed refinement models which affect coefficients of the correction terms [90, 91].

This has led so far to several indications, while a complete evaluation of the cosmological phenomenology remains to be done. It has been shown that quantum corrections can add up in long cosmological regimes, magnifying potentially visible effects [85]. The scalar mode equations can be combined with a quantum-corrected Poisson equation, whose classical solution would be the Newton potential. Thus, this line of research allows a derivation of the Newton potential in a classical limit of quantum gravity together with a series of corrections. This offers interesting comparisons with the spin-foam approach to the graviton propagator [257]. Although the formulations are quite different, there are some similarities, e.g., in the role of semiclassical states in both approaches; compare, e.g., [216].

4.19.6 Realistic equations of state

Due to quantum corrections to matter Hamiltonians, equations of state of matter change in loop cosmology, which by itself can have cosmological effects. The main example is that of a scalar field, whose effective density and pressure directly provide the equation of state. Similarly, one can easily derive equations of state for some perfect fluid models, such as dust ($w = 0$). In this case, the total energy is just a field-independent constant, which remains a simple constant as a contribution to the simple quantum Hamiltonian. The dust equation of state thus receives no quantum corrections. (Note that it is important that the Hamiltonian is quantized, not energy density, for which no analog in the full theory would exist. For the energy density of dust, one certainly has inverse powers of the scale factor and could thus wrongly expect corrections from loop cosmology; see also [277] for such expressions for other fluids.)

A derivation of effective equations of state is more indirect for other perfect fluids since a fundamental realization through a field is required for a loop quantization. This can be done for the radiation equation of state $w = \frac{1}{3}$ since it is a result of the Maxwell Hamiltonian of the electromagnetic field. Here, one is required to use an inhomogeneous setting in order to have a non-trivial field. Techniques to derive quantum-corrected equations of state thus resemble those used for cosmological perturbation theory. The Hamiltonian derivation of the equation of state, including inverse volume corrections in loop quantum cosmology, can be found in [77]. A similar derivation for relativistic fermions, which obey the same equation of state, is given in [78].

4.19.7 Big Bang nucleosynthesis

Big Bang nucleosynthesis takes place at smaller energy densities than earlier stages of the Big Bang, but there are rather tight constraints on the behavior of different types of matter, radiation and fermions during this phase. Thus, this might provide another handle on quantum-gravity phenomenology, or at least present a phase where one has to make sure that quantum gravity already behaves classically enough to be consistent with observations.

For a detailed analysis, equations of state are required for both the Maxwell fields and fermions. The latter can be assumed to be massless at those energies and thus relativistic, so that all matter fields classically satisfy the equation of state $P = \frac{1}{3}\rho$. However, their Hamiltonians receive quantum corrections in loop quantum gravity, which could lead to different equations of state for the two types of fields, or, in any case, to corrections that may be common to both fields. Any such correction may upset the fine balance required for successful Big Bang nucleosynthesis, and thus puts limits on parameters of loop quantum gravity.

Corrections for the equation of state of radiation have been computed in [77]. Fermions are more difficult to quantize, and the necessary steps are dispersed over several articles. Their kinematics can be found in [32, 289], where [289] introduces half-densitized fermions, which play a key role in consistent quantization. Dynamics, i.e., the definition of Hamiltonian constraint operators, is also discussed in [289] as well as in older work [235, 234, 236]; however, torsion, which inevitably occurs for connection theories of gravity in the presence of fermions, was not included. This is completed in the full treatment of Dirac fermions, starting from an analysis of the Holst-Dirac action [183], provided in [76]. One can take the resulting canonical quantization in the presence of torsion as a starting point for quantum corrections to the fermion equation of state [78]. Applications to Big Bang nucleosynthesis [78] have provided some bounds on parameters, which can play a role once more information about the precise dynamics of inhomogeneous quantum states has been obtained. This application has also highlighted the need for understanding the role of the thermodynamics of a system on a quantum corrected spacetime. From effective loop cosmology one can derive corrections to the energy density $\rho(a)$ or equation of state, but additional input is needed for energy density $\rho(T)$ as a function of temperature as it often occurs. Such considerations of matter thermodynamics on a quantum spacetime have just started.

4.20 Summary

Loop cosmology is a phenomenological description of quantum effects in cosmology, obtained in the framework of a background independent and non-perturbative quantization. There are different types of quantum corrections to classical equations: effective densities in matter Hamiltonians or the gravitational part of the Hamiltonian constraint, higher powers of extrinsic curvature, and quantum backreaction effects. While the former two correspond directly to discreteness effects of quantum geometry, the latter is a genuine quantum effect. Effective density corrections have a non-perturbative component as they contain inverse powers of the Planck length and thus the gravitational constant, while purely perturbative corrections arise from extrinsic curvature terms. Quantum backreaction has not yet been studied systematically except for special models.

These corrections are responsible for a surprising variety of phenomena, which all improve the behavior in classical cosmology. Nevertheless, they were not motivated by phenomenology but were derived through background-independent quantization. In most models and applications the corrected equations introduce different geometrical effects separately, rather than proceeding with complete effective equations including all quantum corrections. In this sense, such studies are phenomenological since they isolate specific effects. While some situations have already been supported by the rigorous effective equations discussed in Section 6, such a justification remains to be worked out in general; see [110] for a general discussion. Once all corrections are included, one has complete effective equations in a strict sense. This has been achieved so far only in one class of models; see Section 6.3. Most currently available models are incomplete but provide a wide range of perturbative calculations and have passed several non-trivial tests for consistent behavior.

Details of the derivation in cosmological models and of their technical origin will now be reviewed in Section 5, before we come to precise effective equations in Section 6 and a discussion of the link to the full theory in Section 7.

5 Loop Quantization of Symmetric Models

Analogies prove nothing, but they can make one feel more at home.

Sigmund Freud
Introductory Lectures on Psychoanalysis

In full loop quantum gravity, the quantum representation is crucial for the foundation of the theory. The guiding theme there is background independence, which requires one to smear the basic fields in a particular manner to holonomies and fluxes. In this section, we will see what implications this has for composite operators and the physical effects they entail. We will base this analysis on symmetric models in order to be able to perform explicit calculations.

Symmetries are usually introduced in order to simplify calculations or make them possible in the first place. However, symmetries can sometimes also lead to complications in conceptual questions, if the additional structure they provide is not fully taken into account. In the present context, it is important to realize that the action of a symmetry group on a space manifold provides a partial background such that the situation is always slightly different from the full theory. If the symmetry is strong, such as in homogeneous models, other representations such as the Wheeler–DeWitt representation can be possible even though the fact that a background has been used may not be obvious. While large-scale physics is not very sensitive to the representation used, it becomes very important on the smallest scales, which we have to take into account when the singularity issue is considered.

Instead of looking only at one symmetric model, where one may have different choices for the basic representation, one should keep the full view of different models as well as the full theory. In fact, in loop quantum gravity it is possible to relate models and the full theory such that symmetric states and basic operators, and thus the representation, can be derived from the unique background-independent cyclic representation of the full theory. We will describe this in detail in Section 7, after having discussed the construction of quantum models in the present section. Without making use of the relation to the full theory, one can construct models by *analogy*. This means that quantization steps are modeled on those, which are known to be crucial in the full theory, which start with the basic representation and continue to the Hamiltonian constraint operator. One can then disentangle the places where additional input, in comparison to the full theory, is needed and what implications it may have.

5.1 Symmetries and backgrounds

It is impossible to introduce symmetries in a completely background-independent manner. The mathematical action of a symmetry group is defined by a mapping between abstract points, which do not exist in a diffeomorphism-invariant setting (if one, for instance, considers only equivalence classes up to arbitrary diffeomorphisms).

More precisely, while the full theory has as background only a differentiable or analytic manifold Σ, a symmetric model has as background a symmetric manifold (Σ, S) consisting of a differentiable or analytic manifold Σ together with an action of a symmetry group $S\colon \Sigma \to \Sigma$. How strong the additional structure is depends on the symmetry used. The strongest symmetry in gravitational models is realized with spatial isotropy, which implies a unique spatial metric up to a scale factor. The background is thus equivalent to a conformal space.

All constructions in a given model must take its symmetry into account since otherwise its particular dynamics, for instance, could not be captured. The structure of models thus depends on the different types of background realized for different symmetry groups. This can not only lead to simplifications but also to conceptual differences, and it is always instructive to keep a complete view on different models as well as the full theory. Since the loop formalism is general enough to encompass all relevant models, there are many ways to compare and relate different systems. It is thus possible to observe characteristic features of (metric) background independence even in cases where more structure is available.

5.2 Isotropy

Isotropic models are described purely in terms of the scale factor $a(t)$ such that there is only a single kinematical degree of freedom. In connection variables, this is parameterized by the triad component p conjugate to the connection component c.

If we restrict ourselves to the invariant connections of a given form, it suffices to probe them with only special holonomies. For an isotropic connection $A_a^i = \tilde{c}\Lambda_I^i\omega_a^I$ (see Appendix B.2) we can choose holonomies along one integral curve of a symmetry generator X_I. They are of the form

$$h_I = \exp(\textstyle\int A_a^i X_I^a \tau_i) = \cos(\frac{1}{2}\mu c) + 2\Lambda_I^i\tau_i \sin(\frac{1}{2}\mu c), \tag{44}$$

where μ depends on the parameter length of the curve and can be any real number (thanks to homogeneity, path ordering is not necessary). Since knowing the values of $\cos(\frac{1}{2}\mu c)$ and $\sin(\frac{1}{2}\mu c)$ for all μ uniquely determines the value of c, which is the only gauge-invariant information contained in the connection, these holonomies describe the configuration space of connections completely.

This illustrates how symmetric configurations allow one to simplify the constructions behind the full theory. But it also shows what effects the presence of a partial background can have on the formalism [16]. In the present case, the background enters through the left-invariant 1-forms ω^I defined on the spatial manifold, whose influence is condensed in the parameter μ. All information about the edge used to compute the holonomy is contained in this single parameter, which leads to degeneracies in comparison to the full theory. Most importantly, one cannot distinguish between the parameter length and the spin label of an edge: Taking a power of the holonomy in a non-fundamental representation simply rescales μ, which could just as well come from a longer parameter length. That this is related to the presence of a background can be seen by looking at the role of edges and spin labels in the full theory. There, both concepts are independent and appear very differently. While the embedding of an edge, including its parameter length, is removed by diffeomorphism invariance, the spin label remains well defined and is important for ambiguities of operators. In the model, however, the full diffeomorphism invariance is not available, such that some information about edges remains in the theory and merges with the spin label. One can see in detail how the degeneracy arises in the process of inducing the representation of the symmetric model [66]. Issues like that have to be taken into account when constructing operators in a model and comparing with the full theory.

The functions appearing in holonomies for isotropic connections define the algebra of functions on the classical configuration space, which, together with fluxes, is to be represented on a Hilbert space. This algebra does not contain arbitrary continuous functions of c but only almost periodic ones of the form [16]

$$f(c) = \sum_\mu f_\mu \exp(i\mu c/2) \tag{45}$$

where the sum is over a countable subset of $\mathbb{R}$. This is analogous to the full situation, reviewed in Section 3.4, where matrix elements of holonomies define a special algebra of continuous functions of connections. As in this case, the algebra is represented as the set of *all* continuous functions on a compact space, called its spectrum. This compactification can be imagined as being obtained from enlarging the classical configuration space $\mathbb{R}$ by adding points, and thus more continuity conditions, until only functions of the given algebra survive as continuous ones. A well-known example is the one point compactification, which is the spectrum of the algebra of continuous functions f for which $\lim_{x\to-\infty} f(x) = \lim_{x\to\infty} f(x)$ exists. In this case, one just needs to add a single point at infinity.

In the present case, the procedure is more complicated and leads to the Bohr compactification $\overline{\mathbb{R}}_{\mathrm{Bohr}}$, which contains $\mathbb{R}$ densely. It is very different from the one-point compactification, as can be seen from the fact that the only functions that are continuous on both spaces are constants. In contrast to the one-point compactification, the Bohr compactification is an Abelian group, just like $\mathbb{R}$ itself. Moreover, there is a one-to-one correspondence between irreducible representations of $\mathbb{R}$ and irreducible representations of $\overline{\mathbb{R}}_{\mathrm{Bohr}}$, which can also be used as the definition of the Bohr compactification. Representations of $\overline{\mathbb{R}}_{\mathrm{Bohr}}$ are thus labeled by real numbers and given by $\rho_\mu\colon \overline{\mathbb{R}}_{\mathrm{Bohr}} \to \mathbb{C}, c \mapsto e^{i\mu c}$. As with any compact group, there is a unique normalized Haar measure $\mathrm{d}\mu(c)$ given explicitly by

$$\int_{\overline{\mathbb{R}}_{\mathrm{Bohr}}} f(c)\,\mathrm{d}\mu(c) = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} f(c)\,\mathrm{d}c\,, \tag{46}$$

where on the right-hand side the Lebesgue measure on $\mathbb{R}$ is used. (For further details of the Bohr compactification and the Hilbert space representation it defines, see ,e.g., [165].)

The Haar measure defines the inner product for the Hilbert space $L^2(\overline{\mathbb{R}}_{\mathrm{Bohr}}, \mathrm{d}\mu(c))$ of square integrable functions on the quantum configuration space. As one can easily check, exponentials of the form $\langle c|\mu\rangle = e^{i\mu c/2}$ are normalized and orthogonal to each other for different μ,

$$\langle\mu_1|\mu_2\rangle = \delta_{\mu_1,\mu_2}\,, \tag{47}$$

which demonstrates that the Hilbert space is not separable.

Similar to holonomies, one needs to consider fluxes only for special surfaces, and all information is contained in the single number p. Since it is conjugate to c, it is quantized to a derivative operator

$$\hat{p} = -\tfrac{1}{3} i\gamma\ell_{\mathrm{P}}^2 \frac{\mathrm{d}}{\mathrm{d}c}\,, \tag{48}$$

whose action

$$\hat{p}|\mu\rangle = \tfrac{1}{6}\gamma\ell_{\mathrm{P}}^2\mu|\mu\rangle =: p_\mu|\mu\rangle \tag{49}$$

on basis states $|\mu\rangle$ can easily be determined. In fact, the basis states are eigenstates of the flux operator, which demonstrates that the flux spectrum is discrete (all eigenstates are normalizable).

This property is analogous to the full theory with its discrete flux spectra and, similarly, it implies discrete quantum geometry. We thus see that the discreteness survives the symmetry reduction in this framework [45]. Likewise, the fact that only holonomies are represented in the full theory, but not connection components, is realized in the model, too. In fact, we have so far represented only exponentials of c, and one can see that these operators are not continuous in the parameter μ. Thus, an operator quantizing c directly does not exist on the Hilbert space. These properties are analogous to the full theory, but very different from the Wheeler–DeWitt quantization. In fact, the resulting representations in isotropic models are inequivalent. While the representation is not of crucial importance when only small energies or large scales are involved [19], it becomes essential at small scales, which are found frequently in cosmology.

5.3 Isotropy: Matter Hamiltonian

We now know how the basic quantities p and c are quantized, and can use the operators to construct more complicated ones. Of particular importance, as well as for cosmology, are matter Hamiltonians, where not only the matter field but also geometry is quantized. For an isotropic geometry and a scalar, this requires us to quantize $|p|^{-3/2}$ for the kinetic term and $|p|^{3/2}$ for the potential term. The latter can be readily defined as $|\hat{p}|^{3/2}$, but for the former we need an inverse power of p. Since $\hat{p}$ has a discrete spectrum containing zero, a densely-defined inverse does not exist.

At this point, one has to find an alternative route to the quantization of $d(p) = |p|^{-3/2}$, or else one could only conclude that there is no well-defined quantization of matter Hamiltonians as a manifestation of the classical divergence. In the case of loop quantum cosmology it turns out, following a general scheme of the full theory [291], that one can reformulate the classical expression in an equivalent way such that quantization becomes possible. One possibility is to write, similar to Equation (13),

$$d(p) = \left(\frac{1}{3\pi\gamma G}\sum_{I=1}^{3}\mathrm{tr}\left(\tau_I h_I\{h_I^{-1},\sqrt{V}\}\right)\right)^6,$$

where we use holonomies of isotropic connections and the volume $V = |p|^{3/2}$. In this expression we can insert holonomies as multiplication operators and the volume operator, and turn the Poisson bracket into a commutator. The result

$$\widehat{d(p)} = \left(8i\gamma^{-1}\ell_{\mathrm{P}}^{-2}(\sin\tfrac{1}{2}c\sqrt{\hat{V}}\cos\tfrac{1}{2}c - \cos\tfrac{1}{2}c\sqrt{\hat{V}}\sin\tfrac{1}{2}c)\right)^6 \tag{50}$$

is not only a densely defined operator but even bounded, which one can easily read off from the eigenvalues [49]

$$\widehat{d(p)}|\mu\rangle = \left(4\gamma^{-1}\ell_{\mathrm{P}}^{-2}(\sqrt{V_{\mu+1}} - \sqrt{V_{\mu-1}}\,)\right)^6|\mu\rangle \tag{51}$$

with $V_\mu = |p_\mu|^{3/2}$ and p_μ from Equation (49).

Rewriting a classical expression in such a manner can always be done in many equivalent ways, which in general all lead to different operators. In the case of $|p|^{-3/2}$, we highlight the choice of the representation in which to take the trace (understood as the fundamental representation above) and the power of $|p|$ in the Poisson bracket ($\sqrt{V} = |p|^{3/4}$ above). This freedom can be parameterized by two ambiguity parameters $j \in \frac{1}{2}\mathbb{N}$ for the representation and $0 < l < 1$ for the power such that

$$d(p) = \left(\frac{3}{8\pi\gamma Glj(j+1)(2j+1)}\sum_{I=1}^{3}\mathrm{tr}_j(\tau_I h_I\{h_I^{-1},|p|^l\})\right)^{3/(2-2l)}.$$

Following the same procedure as above, we obtain eigenvalues [55, 58]

$$\widehat{d(p)}_{j,l}^{(\mu)} = \left(\frac{9}{\gamma\ell_{\mathrm{P}}^2 lj(j+1)(2j+1)}\sum_{k=-j}^{j}k|p_{\mu+2k}|^l\right)^{3/(2-2l)},$$

which, for larger j, can be approximated by Equation (26) (see also Figure 9). This provides the basis for effective densities in loop cosmology as described in Section 4.

Notice that operators for the scale factor, volume or their inverse powers do not refer to observable quantities. It can thus be dangerous, though suggestive, to view their properties as possible bounds on curvature. The importance of operators for inverse volume comes from the fact that this appears in matter Hamiltonians, and thus the Hamiltonian constraint of gravity. Properties of those operators such as their boundedness or unboundedness can then determine the dynamical behavior (see, e.g., [62]).

5.4 Isotropy: Hamiltonian constraint

Dynamics is controlled by the Hamiltonian constraint, which classically gives the Friedmann equation. Since the classical expression (29) contains the connection component c, we have to use

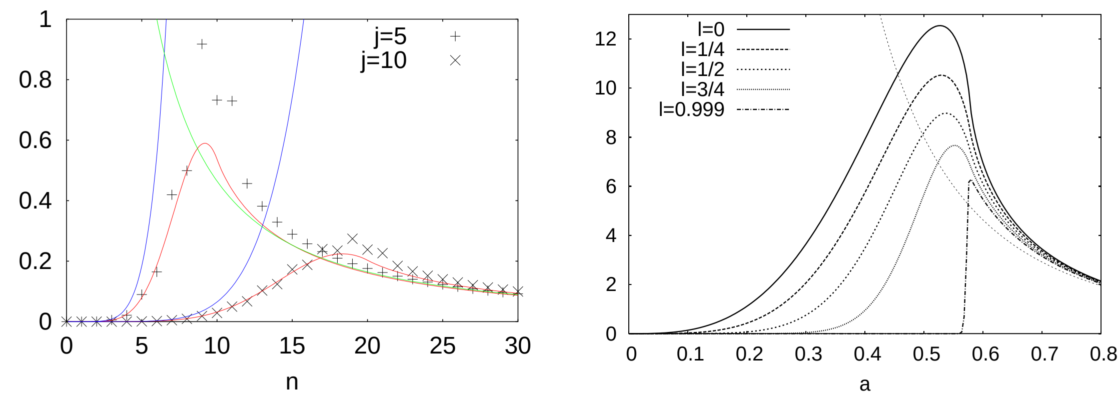

Figure 9: Discrete subset of eigenvalues of $\widehat{d(p)}$ (left) for two choices of j (and $l = \frac{3}{4}$), together with the approximation $d(p)_{j,l}$ from Equation (26) and small-p power laws. The classical divergence at small p, where the behavior differs strongly from eigenvalues, is cut off. The right panel shows the dependence of the initial increase on l.

holonomy operators. In quantum algebra we have only almost-periodic functions at our disposal, which does not include polynomials such as c^2. Quantum expressions can, therefore, only coincide with the classical one in appropriate limits, which in isotropic cosmology is realized for small extrinsic curvature, i.e., small c in the flat case. We thus need an almost periodic function of c, which for small c approaches c^2. This can easily be found, e.g., the function $\sin^2 c$. Again, the procedure is not unique since there are many such possibilities, e.g., $\delta^{-2} \sin^2 \delta c$, and more quantization ambiguities ensue. In contrast to the density $|p|^{-3/2}$, where we also used holonomies in the reformulation, the expressions are not equivalent to each other classically, but only in the small-curvature regime. As we will discuss shortly, the resulting new terms have the interpretation of higher-order corrections to the classical Hamiltonian.

One can restrict the ambiguities to some degree by modeling the expression on that of the full theory. This means that one does not simply replace c^2 by an almost periodic function, but uses holonomies tracing out closed loops formed by symmetry generators [50, 54]. Moreover, the procedure can be embedded in a general scheme that encompasses different models and the full theory [292, 50, 68], further reducing ambiguities. In particular models with non-zero intrinsic curvature on their symmetry orbits, such as the closed isotropic model, can then be included in the construction. (There are different ways to do this consistently, with essentially identical results; compare [111] with [28] for the closed model and [300] with [285] for $k = -1$.) One issue to keep in mind is the fact that "holonomies" are treated differently in models and the full theory. In the latter case they are ordinary holonomies along edges, which can be shrunk and then approximate connection components. In models, on the other hand, one sometimes uses direct exponentials of connection components without integration. In such a case, connection components are reproduced in the corrections only when they are small. Alternatively, a scale-dependent $\delta(\mu)$ can provide the suppression even if connection components remain large in semiclassical regimes. The requirement that this happens in an acceptable way provides restrictions on refinement models, especially if one goes beyond isotropy. Selecting refinement models, on the other hand, leads to important feedback for the full theory. The difference between the two ways of dealing with holonomies can be understood in inhomogeneous models, where they are both realized for different connection components.

In the flat case the construction is easiest, related to the Abelian nature of the symmetry group. One can directly use the exponentials h_I in (44), viewed as 3-dimensional holonomies along integral curves, and mimic the full constraint where one follows a loop to get curvature components of the connection A_a^i. Respecting the symmetry, this can be done in the model with a square loop in two independent directions I and J. This yields the product $h_I h_J h_I^{-1} h_J^{-1}$, which appears in a trace as in Equation (15), together with a commutator $h_K[h_K^{-1}, \hat{V}]$, using the remaining direction K. The latter, following the general scheme of the full theory reviewed in Section 3.6, quantizes the contribution $\sqrt{|p|}$ to the constraint, instead of directly using the simpler $\sqrt{|\hat{p}|}$.

Taking the trace one obtains a diagonal operator

$$\sin(\tfrac{1}{2}\delta c)\hat{V}\cos(\tfrac{1}{2}\delta c) - \cos(\tfrac{1}{2}\delta c)\hat{V}\sin(\tfrac{1}{2}\delta c)$$

in terms of the volume operator, as well as the multiplication operator

$$\sin^2(\tfrac{1}{2}\delta c)\cos^2(\tfrac{1}{2}\delta c) = \sin^2(\delta c), \tag{52}$$

as the only term resulting from $h_I h_J h_I^{-1} h_J^{-1}$ in $\mathrm{tr}(h_I h_J h_I^{-1} h_J^{-1} h_K[h_K^{-1}, \hat{V}])$. In the triad representation, where instead of working with functions $\langle c|\psi\rangle = \psi(c)$ one works with the coefficients ψ_μ in an expansion $|\psi\rangle = \sum_\mu \psi_\mu|\mu\rangle$, this operator is the square of a difference operator. The constraint equation thus takes the form of a difference equation

$$\begin{aligned}(V_{\mu+5\delta} - V_{\mu+3\delta})e^{ik}\psi_{\mu+4\delta}(\phi) - (2 + k\gamma^2\delta^2)(V_{\mu+\delta} - V_{\mu-\delta})\psi_\mu(\phi)\\ + (V_{\mu-3\delta} - V_{\mu-5\delta})e^{-ik}\psi_{\mu-4\delta}(\phi) = -\frac{16\pi}{3}G\gamma^3\delta^3\ell_{\mathrm{P}}^2\hat{H}_{\mathrm{matter}}(\mu)\psi_\mu(\phi)\end{aligned} \tag{53}$$

for the wave function ψ_μ, which can be viewed as an evolution equation in internal time μ. Thus, discrete spatial geometry implies a discrete internal time [51]. The equation above results in the most direct path from a non-symmetric constraint operator with gravitational part acting as

$$\hat{H}|\mu\rangle = \frac{3}{16\pi G\gamma^3\delta^3\ell_{\mathrm{P}}^2}(V_{\mu+\delta} - V_{\mu-\delta})(e^{-ik}|\mu+4\delta\rangle - (2 + k^2\gamma^2\delta^2)|\mu\rangle + e^{ik}|\mu-4\delta\rangle)\,. \tag{54}$$

Operators of this form are derived in [54, 16] for a spatially-flat model ($k = 0$), in [111, 28, 286] for positive spatial curvature ($k = 1$), and in [300, 285] for negative spatial curvature ($k = -1$), which is not included in the forms of Equations (53) and (54). Note, however, that not all these articles used the same quantization scheme and thus operators even for one model appear different in details, although the main properties are the same. Some of the differences of quantization schemes will be discussed below. The main option in alternative quantizations relates to a possible scale dependence $\delta(\mu)$, which we leave open at this stage.

One can symmetrize this operator and obtain a difference equation with different coefficients, which we do here after multiplying the operator with $\mathrm{sign}(\widehat{p})$ for reasons that will be discussed in the context of singularities in Section 5.16. The resulting difference equation is

$$\begin{aligned}(|\Delta_\delta V|(\mu+4\delta) + |\Delta_\delta V|(\mu))e^{ik}\psi_{\mu+4\delta}(\phi) - 2(2 + k^2\gamma^2\delta^2)|\Delta_\delta V|(\mu)\psi_\mu(\phi)\\ + (|\Delta_\delta V|(\mu-4\delta) + |\Delta_\delta V|(\mu))e^{-ik}\psi_{\mu-4\delta}(\phi) = -\frac{32\pi}{3}G\gamma^3\delta^3\ell_{\mathrm{P}}^2\hat{H}_{\mathrm{matter}}(\mu)\psi_\mu(\phi)\end{aligned} \tag{55}$$

where $|\Delta_\delta V|(\mu) := \mathrm{sgn}(\mu)(V_{\mu+\delta} - V_{\mu-\delta}) = |V_{\mu+\delta} - V_{\mu-\delta}|$.

Since $\sin c|\mu\rangle = -\frac{1}{2}i(|\mu+2\rangle - |\mu-2\rangle)$, the difference equation is of higher order, even formulated on an uncountable set, and thus has many independent solutions if δ is constant. Most of them, however, oscillate on small scales, i.e., between μ and $\mu + m\delta$ with small integer m. Others oscillate only on larger scales and can be viewed as approximating continuum solutions. For non-constant δ, we have a difference equation of non-constant step size, where it is more complicated to analyze the general form of solutions. (In isotropic models, however, such equations can always be transformed to equidistant form up to factor ordering [75].) As there are quantization choices, the behavior of all the solutions leads to possibilities for selection criteria of different versions of the constraint. Most importantly, one chooses the routing of edges to construct the square holonomy, again the spin of a representation to take the trace [170, 299], and factor-ordering choices between quantizations of c^2 and $\sqrt{|p|}$. All these choices also appear in the full theory, such that one can draw conclusions for preferred cases there.

5.5 Dynamical refinements of the discreteness scale

Although basic holonomies depend only on the connection, the Hamiltonian constraint operator may in principle contain almost periodic functions of connection components with a coefficient δ depending on the scale μ. Since the step size of the difference equation is determined by this coefficient, the equation will no longer be of constant step size. While such behavior in general makes an analysis of the equation more complicated, there are advantages for the viability of specific solutions, if the discreteness becomes smaller for large volume. In some models, problems can indeed arise if the step size of the difference equation stays constant in the triad component, i.e., in μ, in particular in the presence of a cosmological constant [54]. Several other issues related to such effects have been discussed recently in isotropic models [27], anisotropic ones [75] and in phenomenological applications [240, 239, 90, 91].

While it was expected early on that inhomogeneous situations would provide a refinement of the discreteness scale at larger volumes, a direct derivation from the full theory remains out of reach and the overall status is still at a somewhat heuristic level. Nevertheless, within models one can test different versions of refinements for their viability, which then also provides valuable feedback for the full dynamical behavior. For such reasons it was suggested in [27] that one build in a scale dependence of the discreteness by hand, simply postulating that $\delta(\mu)$ has a certain, non-constant form. The specific behavior, $\delta \propto |\mu|^{-1/2}$, proposed in [27], was argued to have some aesthetic advantages, but other functional forms are possible, too.[2] In fact, considerations of inhomogeneous constraint operators suggest a behavior of the form $\delta \propto |\mu|^x$ with $0 < x < -1/2$. In this class, the case of constant step size in μ ($x = 0$) and the proposal of [27] ($x = -1/2$) appear as limiting cases. A value of x near $-1/2$ currently seems preferred by several independent arguments [75, 240, 91]. (Quantizations for different x are not related by unitary transformations, and one can indeed expect physical arguments to distinguish between different values. Some non-physical arguments have been proposed which aim to fix $x = -1/2$ from the outset, mainly based on the observation that this case makes holonomy corrections to effective equations independent of the parameter V_0 used in the formulation of homogeneity (Section 4.2). This argument is flawed, however, because (i) effective densities will nevertheless depend on V_0, (ii) the quantization is still not invariant because it depends on the coefficient in the proportionality $\delta \propto |\mu|^{-1/2}$ (sometimes called the area gap) and (iii) while for isotropic models a semiclassically suitable value for x results from this argument, the situation is more complicated in anisotropic models. As we will see in the discussion of inhomogeneous situations in Section 6.4, the V_0-dependence results from the minisuperspace reduction, rather than from a gauge artifact, as is sometimes claimed. It can only be understood properly in the relation between homogeneous and inhomogeneous models. For this,

[2] The main motivation in [27] was the use of geometrical rather than coordinate areas to quantize curvature components of the Ashtekar connection via holonomies around closed loops. The geometrical area, measured through the dynamical densitized triad p, then introduces the scale dependence in holonomies appearing in the Hamiltonian constraint. However, this procedure appears somewhat ad hoc because (i) single curvature components quantized through holonomies by Equation (14) refer to coordinates and thus the coordinate area is, in fact, more natural than an invariant geometrical area, and (ii) the quantization then requires the use of the area operator in the Hamiltonian constraint, which is not understood in the full theory. Thus, the original motivation of [27] refers to an argument within the model but not mirrored in the full theory, and thus is suspicious. In Section 6.4 we will discuss a more direct argument [66] for a scale-dependent discreteness suggested by typical properties of the full dynamics.

only the algebra of basic operators is needed, which is also under good control in inhomogeneous settings, as described in Section 7.)

With a scale-dependent discreteness, the continuum limit can be approached dynamically rather than as a mathematical process. While the universe expands, the discreteness is being refined and thus wave functions at large volume are supported on much finer lattices than at small volume. It is clear that this is relevant for the semiclassical limit of the theory, which should be realized for a large universe. Moreover, the relation to dynamics ties in fundamental constraint operators with low-energy behavior and phenomenology. Thus, studying such refinements results in restrictions for admissible fundamental constraints and can reduce possible quantization ambiguities. On the other hand, a scale-dependent discreteness implies more complicated difference equations. In isotropic models one can always transform the single variable μ and change the factor ordering of the constraint operator in such a way that one obtains an equidistant difference equation in the new variable [75]. Otherwise, if models are anisotropic or even inhomogeneous, this is possible only in special cases, which require new analytical or numerical tools. (See [262] for a numerical procedure.)

5.6 Semiclassical limit and correction terms

When replacing c^2 by holonomies we have amended the constraint as a function on the classical phase space by higher powers of the connection. This is necessary since otherwise the function cannot be quantized, but is different from the quantization of densities because now the replacements are not equivalent to the original constraint classically (although the corrections are small in small curvature regimes, where the classical theory can be trusted). In addition, the limit $\lim_{\delta\to 0}\delta^{-2}\sin^2\delta c$, which would give the classical result, does not exist at the operator level.

This situation is different from the full theory, which is again related to the presence of a partial background [16]. There, the parameter length of edges used to construct appropriate loops is irrelevant and thus can shrink to zero. In the model, however, changing the edge length with respect to the background does change the operator and the limit does not exist. Intuitively, this can be understood as follows: The full constraint operator (15) is a vertex sum obtained after introducing a discretization of space used to choose loops α_{IJ}. This classical regularization sums over all tetrahedra in the discretization, whose number diverges in the limit where the discretization size shrinks to zero. In the quantization, however, almost all these contributions vanish, since a tetrahedron must contain a vertex of a state in order to contribute non-trivially. The result is independent of the discretization size, once it is fine enough, and the limit can thus be taken trivially.

In a homogeneous model, on the other hand, contributions from different tetrahedra of the triangulation must be identical, owing to homogeneity. The coordinate size of tetrahedra drops out of the construction in the full background-independent quantization, as emphasized in Section 3.6, which is part of the reason for the discretization independence. In a homogeneous configuration the number of contributions thus increases in the limit, but their size does not change. This results in an ill-defined limit, as we have already seen within the model itself.

Therefore the difference between models and the full theory is only a consequence of symmetry and not of different approaches. This will also become clear later in inhomogeneous models, where one obtains a mixture of the two situations; see Section 5.11. Moreover, in the full theory one has a situation similar to symmetric models, if one does not only look at the operator limit when the regularization is removed, but also checks the classical limit on semiclassical states. In homogeneous models, the expression in terms of holonomies implies corrections to the classical constraint when curvature becomes larger. This is in analogy to other quantum field theories, where effective actions generally have higher curvature terms. In the full theory, those correction terms can be seen when one computes expectation values of the Hamiltonian constraint in semiclassical states peaked at classical configurations for the connection and triad. When this classical configuration becomes small in volume or large in curvature, correction terms to the classical constraint arise. In this case, the semiclassical state provides the background with respect to which these corrections appear. In a homogeneous model, the symmetry already provides a partial background such that correction terms can be noticed already for the constraint operator itself.

5.6.1 WKB approximation

There are various procedures for making contact between the difference equation and classical constraints. The most straightforward way is to expand the difference operators in a Taylor series, assuming that the wave function is sufficiently smooth. On large scales, this indeed results in the Wheeler–DeWitt equation as a continuum limit in a particular ordering [52]. From then on, one can use the WKB approximation or Wigner functions as usually. (Wigner functions can be defined directly on the Hilbert space of loop quantum cosmology making use of the Bohr compactification [165].

That this is possible may be surprising because, as just discussed, the continuum limit as $\delta \to 0$ does not exist for the constraint operator. And indeed, the limit of the constraint equation, i.e., the operator applied to a wave function, does not exist in general. Even for a wave function, the limit as $\delta \to 0$ does not exist in general, since some solutions are sensitive to the discreteness and do not have a continuum limit at all. When performing the Taylor expansion we already assumed certain properties of the wave function such as that the continuum limit does exist. This then reduces the number of independent wave functions to that present in the Wheeler–DeWitt framework, subject to the Wheeler–DeWitt equation. That this is possible demonstrates that the constraint, in terms of holonomies, does not have problems with the classical limit.

The Wheeler–DeWitt equation results at leading order, and in addition, higher-order terms arise in an expansion of difference operators in terms of δ or γ. Similarly, after the WKB or other semiclassical approximation, there are correction terms to the classical constraint in terms of γ as well as $\hbar$ [146, 241].

This procedure is intuitive, but it is not suitable for inhomogeneous models where the Wheeler–DeWitt representation becomes ill defined. One can evade this by performing the continuum and semiclassical limit together. This again leads to corrections in terms of γ as well as $\hbar$, which are mainly of the following form [36]: matter Hamiltonians receive corrections through the modified density $d(p)$, and there are similar terms in the gravitational part containing $\sqrt{|p|}$. These are purely from triad coefficients, and similarly, connection components lead to higher-order corrections as well as additional contributions summarized in a quantum geometry potential. A possible interpretation of this potential in analogy to the Casimir effect has been put forward in [185]. A related procedure to extract semiclassical properties from the difference operator, based on the Bohmian interpretation of quantum mechanics, has been discussed in [273, 276].

5.6.2 Effective formulation

In general, one not only expects higher-order corrections for a gravitational action but also higher derivative terms. The situation is then qualitatively different since not only correction terms arise to a given equation, but also new degrees of freedom coming from higher derivatives being independent of lower ones. In a WKB approximation, this could be introduced by parameterizing the amplitude of the wave function in a suitable way, but it has not been fully worked out yet [144]. Quantum degrees of freedom arise because a quantum state is described by a wave function $\psi(q)$, which, compared to a classical canonical pair (q, p), has infinitely many degrees of freedom. The classical canonical pair can be related to expectation values $(\langle\psi|\hat{q}|\psi\rangle, \langle\psi|\hat{p}|\psi\rangle)$, while quantum degrees of freedom appear as higher moments, parameterizable as

$$G^{a,n} = \langle\psi| \left((\hat{q} - \langle\hat{q}\rangle)^{n-a}(\hat{p} - \langle\hat{p}\rangle)^{a}\right)_{\mathrm{Weyl}} |\psi\rangle, \tag{56}$$

where totally symmetric ordering is understood and $2 \leq n \in \mathbb{N}$, $0 \leq a \leq n$. The infinite dimensional space of the expectation values, together with all higher moments, is symplectic and provides a geometrical formulation of quantum mechanics [201, 180, 30]; instead of using linear operators on a Hilbert space, one can formulate quantum mechanics on this infinite-dimensional phase space. It is directly obtained from the Hilbert space, where the inner product defines a metric, as well as a symplectic form, on its linear vector space (which in this way even becomes Kähler).

We thus obtain a quantum phase space with infinitely many degrees of freedom, together with a flow defined by the Schrödinger equation. Operators become functions on this phase space through expectation values. The projection $\pi\colon \mathcal{H} \to \mathbb{R}^2, \psi \mapsto (\langle\psi|\hat{q}|\psi\rangle, \langle\psi|\hat{p}|\psi\rangle)$ defines the quantum phase space as a fiber bundle over the classical phase space with infinite-dimensional fibers. Sections of this bundle can be defined by embedding the classical phase space into the quantum phase space by means of suitable semiclassical states. For a harmonic oscillator such embeddings can be defined precisely by dynamical coherent states, which are preserved by the quantum evolution. This means that the quantum flow is tangential to the embedding of the classical phase space such that it agrees with the classical flow. Moreover, the section can be chosen to be horizontal with respect to a connection, whose horizontal subspaces are by definition symplectically orthogonal to the fibers. This is possible because the harmonic oscillator allows coherent states which do not spread at all during evolution: quantum variables remain constant and thus there is no evolution along the fibers of the quantum phase space.

In more general systems, however, quantum variables do change: states spread and are deformed in other ways in a rather complicated manner, which can also affect the expectation values. This is exactly the phenomenon that gives rise to quantum corrections to classical equations, which one can capture in effective descriptions. In fact, the dynamics of quantum variables provides a means for the systematic derivation of effective equations that are analogous to effective actions but can be computed in a purely canonical way [105, 282, 106]. They can thus be applied to canonical quantum gravity; more details and applications are provided in Section 6. In this way, one can derive a suitable, non-horizontal section of the quantum phase space. In some simple cases, part of the effective dynamics can also be studied by finding a suitable section by inspection of the equations of motion, without explicitly deriving the behavior of quantum fluctuations [309, 17].

Gravity, as a constrained system, also requires one to deal with constraints. One computes the expectation value of the Hamiltonian constraint, i.e., first goes to the effective picture and then solves equations of motion. Otherwise, there would simply be no effective equations left after the constraints have been solved by physical states used in expectation values. This provides the relation between fundamental constraint operators giving rise to difference equations for physical states and effective equations. The terms used in the phenomenological equations, such as those of Section 4, are justified in this way, but one has to keep in mind that a complete analysis of most of the models discussed there remains to be done. There will be additional correction terms due to the backreaction of quantum variables on expectation values, which are more complicated to derive and have rarely been included in phenomenological studies. The status of precise effective equations is described in Section 6.

5.7 Homogeneity

A Hamiltonian formulation is available for all homogeneous models of Bianchi class A [161], which have structure constants C^I_{JK} fulfilling $C^I_{JI} = 0$. The structure constants also determine left-invariant 1-forms ω^I in terms of which one can write a homogeneous connection as $A^i_a = \tilde{\phi}^i_I \omega^I_a$ (see Appendix B.1), where all freedom is contained in the x-independent $\tilde{\phi}^i_I$. A homogeneous densitized triad can be written in a dual form with coefficients $\tilde{p}_i^I$ conjugate to $\tilde{\phi}_I^i$. As in isotropic models, one absorbs powers of the coordinate volume to obtain variables ϕ_I^i and p_i^I.

The kinematics is the same for all class A models, except possibly for slight differences in the diffeomorphism constraint [29, 44]. Connection components define a distinguished triple of SU(2) elements $\tilde{\phi}_I^i \tau_i$, one for each independent direction of space. Holonomies in those directions are then obtained as $h_I^{(\mu_I)} = \exp(\mu_I \phi_I^i \tau_i) \in \mathrm{SU}(2)$ with parameters μ_I for the edge lengths. Cylindrical functions depend on those holonomies, i.e., are countable superpositions of terms $f(h_1^{(\mu_1)}, h_2^{(\mu_2)}, h_3^{(\mu_3)})$. A basis can be written down as spin network states

$$f(h_1^{(\mu_1)}, h_2^{(\mu_2)}, h_3^{(\mu_3)}) = \rho_{j_1}(h_1^{(\mu_1)})^{A_1}_{B_1} \rho_{j_2}(h_2^{(\mu_2)})^{A_2}_{B_2} \rho_{j_3}(h_3^{(\mu_3)})^{A_3}_{B_3} K^{B_1 B_2 B_3}_{A_1 A_2 A_3}$$

where the matrix K specifies how the representation matrices are contracted to a gauge invariant function of ϕ_I^i. There are uncountably many such states for different μ_I and thus the Hilbert space is non-separable. In contrast to isotropic models, the general homogeneous theory is genuinely SU(2) and therefore not much simpler than the full theory for individual calculations.

As a consequence of homogeneity we observe the same degeneracy as in isotropic models where spin and edge length both appear similarly as parameters. Spins are important to specify the contraction K and thus enter, e.g., the volume spectrum. For this one needs to know the spins, and it is not sufficient to consider only products $j_I \delta_I$. On the other hand, there is still a degeneracy of spin and edge length; keeping both j_I and δ_I independent leaves too many parameters. Therefore, it is more difficult to determine what the analog of the Bohr compactification is in this case.

5.8 Diagonalization

The situation simplifies if one considers diagonal models, which is usually also done in classical considerations since it does not lead to much loss of information. In a metric formulation, one requires the metric and its time derivative to be diagonal, which is equivalent to a homogeneous densitized triad $p_i^I = p^{(I)} \Lambda_i^I$ and connection $\phi_I^i = c_{(I)} \Lambda_I^i$ with real numbers c_I and p^I (where coordinate volume has been absorbed as described in Appendix B.1), which are conjugate to each other, $\{c_I, p^J\} = 8\pi\gamma G \delta_I^J$, and internal directions Λ_I^i as in isotropic models [56]. In fact, the kinematics becomes similar to isotropic models, except that there are now three independent copies. The reason for the simplification is that we are able to separate off the gauge degrees of freedom in Λ_I^i from gauge-invariant variables c_I and p^I (except for remaining discrete gauge transformations changing the signs of two of the p^I and c_I together). In a general homogeneous connection, gauge-dependent and gauge-invariant parameters are mixed together in ϕ_I^i, which both react differently to a change in μ_I. This makes it more difficult to discuss the structure of relevant function spaces without assuming diagonalization.

As mentioned, the variables p^I and c_I are not completely gauge invariant since a gauge transformation can flip the sign of two components p^I and c_I while keeping the third fixed. There is thus a discrete gauge group left, and only the total sign $\mathrm{sign}(p^1 p^2 p^3)$ is gauge invariant in addition to the absolute values.

Quantization can now proceed simply by using as Hilbert space the triple product of the isotropic Hilbert space, given by square-integrable functions on the Bohr compactification of the real line. This results in states $|\psi\rangle = \sum_{\mu_1,\mu_2,\mu_3} \psi_{\mu_1,\mu_2,\mu_3} |\mu_1, \mu_2, \mu_3\rangle$ expanded in an orthonormal basis

$$\langle c_1, c_2, c_3 | \mu_1, \mu_2, \mu_3 \rangle = e^{i(\mu_1 c_1 + \mu_2 c_2 + \mu_3 c_3)/2} .$$

Gauge invariance under discrete gauge transformations requires ψ_{μ_1,μ_2,μ_3} to be symmetric under a flip of two signs in μ_I. Without loss of generality one can thus assume that ψ is defined for all real μ_3 but only non-negative μ_1 and μ_2.

Densitized triad components are quantized by

$$\hat{p}^I|\mu_1,\mu_2,\mu_3\rangle = \frac{1}{2}\mu_I\gamma\ell_{\mathrm{P}}^2|\mu_1,\mu_2,\mu_3\rangle\,,$$

which give the volume operator $\hat{V}=\sqrt{|\hat{p}^1\hat{p}^2\hat{p}^3|}$ directly with spectrum

$$V_{\mu_1,\mu_2,\mu_3} = (\tfrac{1}{2}\gamma\ell_{\mathrm{P}}^2)^{3/2}\sqrt{|\mu_1\mu_2\mu_3|}\,.$$

Moreover, after dividing out the remaining discrete gauge freedom the only independent sign in the triad components is given by the orientation $\mathrm{sign}(\hat{p}^1\hat{p}^2\hat{p}^3)$, which again leads to a doubling of the metric minisuperspace with a degenerate subset in the interior, where one of the p^I vanishes.

5.9 Homogeneity: Dynamics

The Hamiltonian constraint can be constructed in the standard manner and its matrix elements can be computed explicitly thanks to the simple volume spectrum after diagonalization. There are holonomy operators for all three directions, and so in the triad representation the constraint equation becomes a partial difference equation for ψ_{μ_1,μ_2,μ_3} in three independent variables. Its (lengthy) form can be found in [56] for the Bianchi I model and in [82] for all other class A models.

Simpler cases arise in locally rotationally-symmetric (LRS) models, where a non-trivial isotropy subgroup is assumed. Here, only two independent parameters μ and ν remain, where only one, e.g., ν can take both signs if discrete gauge freedom is fixed, and the vacuum difference equation is, e.g., for Bianchi I,

$$\begin{aligned}&2\delta\sqrt{|\nu+2\delta|}(\psi_{\mu+2\delta,\nu+2\delta}-\psi_{\mu-2\delta,\nu+2\delta})\\&+\tfrac{1}{2}\left(\sqrt{|\nu+\delta|}-\sqrt{|\nu-\delta|}\right)((\mu+4\delta)\psi_{\mu+4\delta,\nu}-2\mu\psi_{\mu,\nu}+(\mu-4\delta)\psi_{\mu-4\delta,\nu})\\&-2\delta\sqrt{|\nu-2\delta|}(\psi_{\mu+2\delta,\nu-2\delta}-\psi_{\mu-2\delta,\nu-2\delta})\\=&\,0\end{aligned} \tag{57}$$

from the non-symmetric constraint and

$$\begin{aligned}&2\delta\left(\sqrt{|\nu+2\delta|}+\sqrt{|\nu|}\right)(\psi_{\mu+2\delta,\nu+2\delta}-\psi_{\mu-2\delta,\nu+2\delta})\\&+\left(\sqrt{|\nu+\delta|}-\sqrt{|\nu-\delta|}\right)((\mu+2\delta)\psi_{\mu+2\delta,\nu}-\mu\psi_{\mu,\nu}+(\mu-2\delta)\psi_{\mu-2\delta,\nu})\\&-2\delta\left(\sqrt{|\nu-2\delta|}+\sqrt{|\nu|}\right)(\psi_{\mu+2\delta,\nu-2\delta}-\psi_{\mu-2\delta,\nu-2\delta})\\=&\,0\end{aligned} \tag{58}$$

from the symmetric version (see also [14] and [75] for the correction of a typo). This leads to a reduction between fully anisotropic and isotropic models with only two independent variables, and provides a class of interesting systems to analyze effects of anisotropies. In [88], for instance, anisotropies are treated perturbatively around isotropy as a model for the more complicated of inhomogeneities. This shows that non-perturbative equations are essential for the singularity issue, while perturbation theory is sufficient to analyze the dynamical behavior of semiclassical states.

Also here, $\delta(\mu)$ can be scale dependent, resulting in non-equidistant difference equations, which in the case of several independent variables are only rarely transformable to equidistant form [75]. A special case where this is possible is studied in [126].

5.10 Inhomogeneous models

Homogeneous models provide a rich generalization of isotropic ones, but inhomogeneities lead to stronger qualitative differences. To start with, at least at the kinematical level one has infinitely many degrees of freedom and is thus always dealing with field theories. Studying field theoretical implications does not require going immediately to the full theory since there are many inhomogeneous models of physical interest.

We will describe some one-dimensional models with one inhomogeneous coordinate x and two others parameterizing symmetry orbits. A general connection is then of the form (with coordinate dependent 1-forms ω_y and ω_z depending on the symmetry)

$$A = A_x(x)\Lambda_x(x)\,\mathrm{d}x + A_y(x)\Lambda_y(x)\omega_y + A_z(x)\Lambda_z(x)\omega_z + \text{field independent terms} \tag{59}$$

with three real functions $A_I(x)$ and three internal directions $\Lambda_I(x)$ normalized to $\mathrm{tr}(\Lambda_I^2) = -\frac{1}{2}$, which in general are independent of each other. The situation in a given point x is thus similar to general homogeneous models with nine free parameters. Correspondingly, there are not many simplifications from this general form, and one needs analogs of the diagonalization employed for homogeneous models (Section 5.8). What is required mathematically for simplifications to occur is a connection with internally-perpendicular components, i.e., $\mathrm{tr}(\Lambda_I\Lambda_J) = -\frac{1}{2}\delta_{IJ}$ at each point. This arises in different physical situations.

5.11 Einstein–Rosen waves

One class of one-dimensional models is given by cylindrically-symmetric gravitational waves, with connections and triads

$$A = A_x(x)\tau_3\mathrm{d}x + (A_1(x)\tau_1 + A_2(x)\tau_2)\mathrm{d}z + (A_3(x)\tau_1 + A_4(x)\tau_2)\mathrm{d}\varphi \tag{60}$$

$$E = E^x(x)\tau_3\frac{\partial}{\partial x} + (E^1(x)\tau_1 + E^2(x)\tau_2)\frac{\partial}{\partial z} + (E^3(x)\tau_1 + E^4(x)\tau_2)\frac{\partial}{\partial\varphi} \tag{61}$$

in cylindrical coordinates. This form is more restricted than Equation (59), but still not simple enough for arbitrary A_1, A_2, A_3 and A_4. Einstein–Rosen waves [159, 41] are a special example of cylindrical waves subject to the polarization condition $E_2E_4 + E_1E_3 = 0$ for triad components. Since this is a quadratic condition for momenta, the polarization imposed on connection components takes a different form, which is analyzed in [34]. It turns out that this allows simplifications in the quantization analogous to models with internally-perpendicular connection components and is thus similar to diagonalization in a homogeneous model.

5.11.1 Canonical variables

A difference to homogeneous models, however, is that the internal directions of a connection and a triad do not need to be identical, which in homogeneous models with internal directions Λ_I^i is the case as a consequence of the Gauss constraint $\epsilon^{ijk}\phi_I^j p_k^I = 0$. With inhomogeneous fields, now, the Gauss constraint reads

$$E^{x\prime} + A_1E^2 - A_2E^1 + A_3E^4 - A_4E^3 = 0 \tag{62}$$

or, after splitting off norms and internal directions,

$$A_z := \sqrt{A_1^2 + A_2^2}\,, \qquad A_\varphi := \sqrt{A_3^2 + A_4^2} \tag{63}$$

$$\Lambda_z^A := \frac{A_1\tau_1 + A_2\tau_2}{A_z}\,, \qquad \Lambda_\varphi^A := \frac{A_3\tau_1 + A_4\tau_2}{A_\varphi} \tag{64}$$

and analogously E^z, E^φ, Λ_E^z and Λ_E^φ,

$$E^{x\prime} + A_z E^z \sin\alpha + A_\varphi E^\varphi \sin\bar{\alpha} = 0 \tag{65}$$

with $\sin\alpha := -2\mathrm{tr}(\Lambda_z^A \Lambda_E^z \tau_3)$ and $\sin\bar{\alpha} := -2\mathrm{tr}(\Lambda_\varphi^A \Lambda_E^\varphi \tau_3)$. If E^x is not constant, α and $\bar{\alpha}$ cannot both be zero and thus connections and triads have different internal directions.

As a consequence, E^z is not conjugate to A_z anymore, and instead the momentum of A_z is $E^z \cos\alpha$ [60]. This seems to make quantization more complicated since the momenta will be quantized to simple flux operators, but do not directly determine the geometry, such as the volume $V = 4\pi \int \mathrm{d}x \sqrt{|E^x E^z E^\varphi|}$. For this, one would need to know the angle α, which depends on both connections and triads. Moreover, it would not be obvious how to obtain a discrete volume spectrum since volume does not depend only on fluxes.

It turns out that there is a simple canonical transformation, which allows one to work with canonical variables E^z and E^φ playing the role of momenta of $A_z \cos\alpha$ and $A_\varphi \cos\bar{\alpha}$ [109, 34, 35]. This seems to be undesirable, too, since now the connection variables that play an important role for holonomies are modified. That these canonical variables are very natural, however, follows after one considers the structure of spin connections and extrinsic curvature tensors in this model. The new canonical variables are then simply given by $A_z \cos\alpha = \gamma K_z$, $A_\varphi \cos\bar{\alpha} = \gamma K_\varphi$, i.e., proportional to extrinsic curvature components. Thus, in the inhomogeneous model we simply replace connection components with extrinsic curvature in homogeneous directions (note that A_x remains unchanged) while momenta remain elementary triad components. This is part of a broader scheme, which is also important for the Hamiltonian constraint operator (Section 5.15).

5.11.2 Representation

With the polarization condition the kinematics of the quantum theory simplify. Relevant holonomies are given by $h_e(A) = \exp(\frac{1}{2} i \int_e A_x(x) \mathrm{d}x)$ along edges in the one-dimensional manifold and

$$h_v^z(A) = \exp(i\gamma\nu_v K_z(v)), \qquad h_v^\varphi(A) = \exp(i\gamma\mu_v K_\varphi(v))$$

in vertices v with real $\mu_v, \nu_v \geq 0$. Cylindrical functions depend on finitely many of these holonomies, whose edges and vertices form a graph in the one-dimensional manifold. Flux operators, i.e., quantized triad components, act simply by

$$\hat{E}^x(x) T_{g,k,\mu} = \frac{\gamma \ell_{\mathrm{P}}^2}{8\pi} \frac{k_{e^+(x)} + k_{e^-(x)}}{2} T_{g,k,\mu} \tag{66}$$

$$\int_{\mathcal{I}} \hat{E}^z T_{g,k,\mu} = \frac{\gamma \ell_{\mathrm{P}}^2}{4\pi} \sum_{v \in \mathcal{I}} \nu_v T_{g,k,\mu} \tag{67}$$

$$\int_{\mathcal{I}} \hat{E}^\varphi T_{g,k,\mu} = \frac{\gamma \ell_{\mathrm{P}}^2}{4\pi} \sum_{v \in \mathcal{I}} \mu_v T_{g,k,\mu} \tag{68}$$

on a spin network state

$$\begin{aligned} T_{g,k,\mu}(A) &= \prod_{e \in g} \rho_{k_e}(h_e) \prod_{v \in V(g)} \rho_{\mu_v}(\gamma K_\varphi(v)) \rho_{\nu_v}(\gamma K_z(v)) \rho_{k_v}(\beta(v)) \\ &= \prod_{e \in g} \exp\left(\tfrac{1}{2} i k_e \int_e A_x(x) \mathrm{d}x\right) \prod_{v \in V(g)} e^{i\gamma\mu_v K_\varphi(v)} e^{i\gamma\nu_v K_z(v)} e^{i k_v \beta(v)} , \end{aligned} \tag{69}$$

which also depend on the gauge angle β determining the internal direction of Λ_z^E. If we solve the Gauss constraint at the quantum level, the labels k_v will be such that a gauge invariant spin network only depends on the gauge-invariant combination $A_x + \beta'$.

Since triad components now have simple quantizations, one can directly combine them to get the volume operator and its spectrum

$$V_{k,\mu,\nu} = \frac{\gamma^{3/2}\ell_{\mathrm{P}}^3}{4\sqrt{\pi}} \sum_v \sqrt{\mu_v \nu_v |k_{e^+(v)} + k_{e^-(v)}|}\,. \qquad (70)$$

The labels μ_v and ν_v are always non-negative, and the local orientation is given through the sign of edge labels k_e.

Commutators between holonomies and the volume operator will technically be similar to homogeneous models, except that there are more possibilities to combine different edges. Accordingly, one can easily compute all matrix elements of composite operators such as the Hamiltonian constraint. The result is only more cumbersome because there are more terms to keep track of. Again as in diagonal homogeneous cases, the triad representation exists and one can formulate the constraint equation there. Now, however, one has infinitely many coupled difference equations for the wave function since the lapse function is inhomogeneous, providing one difference equation for each vertex. With refinement, only μ_v and ν_v can possibly be scale dependent but not k_e, which gives the representation for a holonomy along an inhomogeneous direction.

There are obvious differences to cases considered previously owing to inhomogeneity. For instance, each edge label can take positive or negative values, or go through zero during evolution, corresponding to the fact that a spatial slice does not need to intersect the classical singularity everywhere. Also the structure of coefficients of the difference equations, though qualitatively similar to homogeneous models, is changed crucially in inhomogeneous models, mainly due to the volume eigenvalues (70). Now, a single edge label k_{e^+}, say, and thus E^x can be zero without volume eigenvalues in neighboring vertices having zero volume.

5.12 Spherical symmetry

For spherically-symmetric models, a connection has the form (Appendix B.3)

$$A = A_x(x)\tau_3\,\mathrm{d}r + (A_1(x)\tau_1 + A_2(x)\tau_2)\,\mathrm{d}\vartheta + (A_1(x)\tau_2 - A_2(x)\tau_1)\sin\vartheta\,\mathrm{d}\varphi + \tau_3\cos\vartheta\,\mathrm{d}\varphi, \qquad (71)$$

whose field-dependent terms automatically have perpendicular internal directions. In this case, it is not diagonalization as in the polarization condition for Einstein–Rosen waves but a non-trivial isotropy subgroup, which leads to this property. The kinematical quantization is then simplified as discussed before, with the only difference being that there is only one type of vertex holonomy

$$h_v(A) = \exp(i\gamma\mu_v K_\varphi(v))$$

as a consequence of a non-trivial isotropy subgroup. The Hamiltonian constraint can again be computed explicitly [109].

Spherically-symmetric models are usually used for applications to non-rotating black holes, but they can also be useful for cosmological purposes. They are particularly interesting as models for the evolution of inhomogeneities as perturbations, which can be applied to gravitational collapse but also to cosmology. In such a context, one often reduces the spherically-symmetric configuration even further by requiring a spatial metric

$$\mathrm{d}s^2 = q_{xx}(x,t)\,\mathrm{d}x^2 + q_{\varphi\varphi}(x,t)\,\mathrm{d}\Omega^2\,,$$

where q_{xx} is related to $q_{\varphi\varphi}$ by $\partial_x\sqrt{q_{xx}} = \sqrt{q_{\varphi\varphi}}$. One example for such a metric is the spatial part of a flat Friedmann–Robertson–Walker spacetime, where $q_{\varphi\varphi}(x,t) = x^2 a(t)^2$. This allows one to study perturbations around a homogeneous spacetime, which can also be done at the quantum level.

5.13 Loop inspired quantum cosmology

The constructions described so far in this section follow all the steps in the full theory as closely as possible. Most importantly, one obtains quantum representations inequivalent to those used in a Wheeler–DeWitt quantization, which results in many further implications. This has inspired investigations where not all the steps of loop quantum gravity are followed, but only the same type of representation, i.e., the Bohr Hilbert space in an isotropic model, is used. Other constructions, based on ADM rather than Ashtekar variables, are then done in the most straightforward way rather than a way suggested by the full theory [188].

In isotropic models the results are similar, but already here one can see conceptual differences. Since the model is based on ADM variables, in particular using the metric and not triads, it is not clear what the additional sign factor $\mathrm{sign}(\mu)$, which is then introduced by hand, means geometrically. In loop quantum cosmology it arose naturally as an orientation of triads, even before its role in removing the classical singularity, to be discussed in Section 5.16, had been noticed. (The necessity of having both signs available is also reinforced independently by kinematical consistency considerations in the full theory [171].) In homogeneous models the situation is even more complicated since sign factors are still introduced by hand, but not all of them are removed by discrete gauge transformations as in Section 5.8 (see [230] as opposed to [14]). Those models are useful to illuminate possible effects, but they also demonstrate how new ambiguities, even with conceptual implications, arise if guidance from a full theory is lost.

In particular, the internal time dynamics is more ambiguous in those models and thus not usually considered. There are then only arguments that the singularity could be avoided through the boundedness of relevant operators [191], but those statements are not generic in anisotropic models [82] or even the full theory [120]. Moreover, even if all curvature quantities could be shown to be bounded, the evolution could still stop (as happens classically where not any singularity is also a curvature singularity). The focus has shifted to an understanding of horizon dynamics in black hole collapse, where not all properties of the quantum representation may be crucial [190, 189, 192].

5.14 Dynamics

> *Because irrational numbers are always the result of calculations, never the result of direct measurement, might it not be possible in physics to abandon irrational numbers altogether and work only with the rational numbers? That is certainly possible, but it would be a revolutionary change. ...*
>
> *At some future time, when much more is known about space and time and the other magnitudes of physics, we may find that all of them are discrete.*
>
> Rudolf Carnap
> An Introduction to the Philosophy of Science

So far we have mainly described the kinematical construction of symmetric models in loop quantum gravity up to the point where the Hamiltonian constraint appears. Since many dynamical issues in different models appear in a similar fashion, we discuss them in this section with a common background. The main feature is that dynamics is formulated by a difference equation, which by itself, compared to the usual appearance of differential equations, implies new properties of evolution. Depending on the model there are different classes, which even within a given model are subject to quantization choices. Yet, since there is a common construction procedure many characteristic features are very general.

Classically, curvature encodes the dynamics of geometry and does so in quantum gravity, too. On the other hand, quantum geometry is most intuitively understood in eigenstates of geometry, e.g., a triad representation if it exists, in which curvature is unsharp. Anyway, only solutions to the Hamiltonian constraint are relevant, which in general are peaked neither on spatial geometry nor on extrinsic curvature. The role of curvature thus has a different, less direct meaning in quantum gravity. Still, it is instructive to quantize classical expressions for curvature in special situations, such as a^{-2} in isotropy. Since the resulting operator is bounded, it has played an influential role in the development of statements regarding the fate of classical singularities.

However, one has to keep in mind that isotropy is a very special case, as emphasized before, and already anisotropic models shed quite a different light on curvature quantities [71]. Isotropy is special because there is only one classical spatial length scale given by the scale factor a, such that intrinsic curvature can only be a negative power, such as a^{-2} just for dimensional reasons. That quantum corrections to this expression are not obvious in this model or others is illustrated by comparing the intrinsic curvature term ka^{-2}, which remains unchanged and thus unbounded in the purely isotropic quantization, with the term coming from a matter Hamiltonian, where the classical divergence of a^{-3} is cut off.

In an anisotropic model we do have different classical scales and thus dimensionally also terms like $a_1 a_2^{-3}$ are possible. It is then not automatic that the quantization is bounded even if a_2^{-3} were to be bounded. As an example of such quantities consider the spatial curvature scalar given by $W(p^1, p^2, p^3)/(p^1 p^2 p^3)$ with W in Equation (40) through the spin-connection components. When quantized and then reduced to isotropy, one does obtain a cutoff to the intrinsic curvature term ka^{-2} as mentioned in Section 4.12, but the anisotropic expression remains unbounded on minisuperspace. The limit to vanishing triad components is direction dependent and the isotropic case picks out a vanishing limit. However, in general this is not the limit taken along dynamical trajectories. Similarly, in the full theory one can show that inverse volume operators are not bounded even, in contrast to anisotropic models, in states where the volume eigenvalue vanishes [120]. However, this is difficult to interpret since nothing is known about its relevance to dynamics; even the geometrical role of spin labels, and thus of the configurations considered, is unclear.

It is then quantum dynamics that is necessary to see what properties are relevant and how degenerate configurations are approached. This should allow one to check if the classical boundary a finite distance away is removed in quantum gravity. This can only happen if quantum gravity provides candidates for a region beyond the classical singularity, and means to probe how to evolve there. The most crucial aim is to prevent incompleteness of spacetime solutions or their quantum replacements. Even if curvature would be finite, by itself it would not be enough since one could not tell if the singularity persists as incompleteness. Only a demonstration of continuing evolution can ultimately show that singularities are absent.

5.15 Dynamics: General construction

Not all steps in the construction of the full constraint can be taken over immediately to a model since symmetry requirements have to be respected. It is thus important to have a more general construction scheme that shows how generic different steps are, and whether or not crucial input in a given symmetric situation is needed.

We have already observed one such issue, which is the appearance of holonomies and also simple exponentials of connection components without integration. This is a consequence of different transformation properties of different connection components in a reduced context. Components along remaining inhomogeneous directions, such as A_x for Einstein–Rosen waves, play the role of connection components in the model, giving rise to ordinary holonomies. Other components, such as A_z and A_φ in Einstein–Rosen waves or all components in homogeneous models, transform as scalars and thus only appear in exponentials without integration. In the overall picture, we have the full theory with only holonomies, homogeneous models with only exponentials, and inhomogeneous models in between where both holonomies and exponentials appear.

Another crucial issue is that of intrinsic curvature encoded in the spin connection. In the full theory, the spin connection does not have any covariant meaning and in fact can be made to vanish locally. In symmetric models, however, some spin connection components can become covariantly well defined, since not all coordinate transformations are allowed within a model. In isotropic models, for instance, the spin connection is simply given by a constant proportional to the curvature parameter. Of particular importance is the spin connection when one considers semiclassical regimes because intrinsic curvature does not need to become small there, in contrast to extrinsic curvature. Since the Ashtekar connection mixes the spin connection and extrinsic curvature, its semiclassical properties can be rather complicated in symmetric models.

The full constraint is based on holonomies around closed loops in order to approximate Ashtekar-curvature components when the loop becomes small in a continuum limit. For homogeneous directions, however, one cannot shrink the loop and instead must work with exponentials of the components. One thus approximates the classical components only when arguments of the exponential are small. If these arguments were always connection components, one would not obtain the right semiclassical properties because those components can remain large. Thus, one must base the construction for homogeneous directions in models on extrinsic curvature components, i.e., subtract off the spin connection from the Ashtekar connection. For inhomogeneous directions, on the other hand, this is not possible since one needs a connection in order to define a holonomy.

At first sight this procedure may seem rather ad hoc and even goes half a step back to ADM variables since extrinsic curvature components are used. However, there are several places where this procedure turns out to be necessary for a variety of independent reasons. We have already seen in Section 5.11 that inhomogeneous models can lead to a complicated volume operator when one insists on using all Ashtekar connection components. When one allows for extrinsic curvature components in the way just described, on the other hand, the volume operator becomes straightforward. This appeared after performing a canonical transformation, which rests non-trivially on the form of inhomogeneous spin connections and extrinsic curvature tensors.

Moreover, in addition to the semiclassical limit used above as justification, one also has to discuss local stability of the resulting evolution equation [79]: since higher-order difference equations have additional solutions, one must ensure that they do not become dominant in order not to spoil the continuum limit. This is satisfied with the above construction, while it is generically violated if one were to use only connection components.

There is thus a common construction scheme available based on holonomies and exponentials. As already discussed, this is responsible for correction terms in a continuum limit, but also gives rise to the constraint equation being a difference equation in a triad representation, whenever it exists. In homogeneous models the structure of the resulting difference equation is clear, but there are different open possibilities in inhomogeneous models. This is intimately related to the issue of anomalies, which also appears only in inhomogeneous models.

Sometimes it is possible to use implications of refinements of the underlying discreteness to suppress large spin-connection components, and thus retain all Ashtekar-connection components even in homogeneous directions. However, the only non-trivial model so far in which this has been constructed is the closed isotropic model. In other models it is more complicated to compute the required holonomies in terms of components of invariant connections, and it is also unclear whether or not specifics of a given model are used too much in such constructions. Fortunately, in the closed model the result does not differ essentially from what is obtained by the general construction scheme.

With a fixed choice, one has to solve a set of coupled difference equations for a wave function on superspace. The basic question then is always what kind of initial or boundary-value problem has to be used in order to ensure the existence of solutions with suitable properties, e.g., in a semiclassical regime. Once this is specified one can already discuss the singularity problem since one needs to find out if initial conditions in one semiclassical regime together with boundary conditions away from classical singularities suffice for a unique solution on all of superspace. A secondary question is how this equation can be interpreted as an evolution equation for the wave function in an internal time. This is not strictly necessary for all purposes and can be complicated owing to the problem of time in general. Nevertheless, when available, an evolution interpretation can be helpful for interpretations.

5.16 Singularities

Il n'est rien de plus précieux que le temps, puisque c'est le prix de l'éternité.

(*There is nothing more precious than time, for it is the price of eternity.*)

Louis Bourdaloue
Sermon sur la perte de temps

In the classical situation, we always have trajectories on superspace running into singular sub-manifolds at which some or all densitized triad components vanish. In semiclassical regimes one can think of physical solutions as wave packets following these trajectories in internal time, but at smaller triad components spreading and deformations from a Gaussian become stronger. Moreover, discreteness becomes essential and properties of difference equations need to be taken into account in order to see what is happening at the singular sub-manifolds.

The simplest situation is given by isotropic models in which superspace is one-dimensional with coordinate p. Minisuperspace is thus disconnected classically with two sides separated by the classical singularity at $p = 0$. (Some singularities occur at $p \neq 0$, such as the "big break" treated with quantum cosmology in [196].) At this point, classical energy densities diverge and there is no well-defined initial-value problem to evolve further. (Sometimes, formal extensions of solutions beyond a classical singularity exist [177], but they are never unique and unrelated to the solution preceding the singularity. This shows that a resolution of singularities has not only to provide a new region, but also an evolution there unique from initial values at one side.) A Wheeler–DeWitt quantization would similarly lead to diverging matter-Hamiltonian operators and the initial-value problem for the wave function generically breaks down. In isotropic loop quantum cosmology we have already seen that the matter Hamiltonian does not have diverging contributions from inverse metric components even at the classical singularity. Nevertheless, the evolution could break down if highest-order coefficients in the difference equation become zero. This indeed happens with the non-symmetric constraint (53) or (57), but in these cases it can be seen not to lead to any problems: some coefficients can become zero such that the wave function at $\mu = 0$ remains undetermined by initial conditions, but the wave function at the other side of the classical singularity is still determined uniquely. There is no breakdown of evolution, and thus no singularity [47]. As one can see, this relies on crucial properties of the loop representation with well-defined inverse metric components and a difference rather than differential equation [51].

In addition, the structure of the difference equations is important, depending on some choices. Most important is the factor ordering or symmetrization chosen. As just discussed, the ordering used earlier leads to non-singular evolution but with the wave function at the classical singularity itself remaining undetermined. In anisotropic models one can symmetrize the constraint and obtain a difference equation, such as Equation (58), whose leading-order coefficients never vanish. Evolution then never stops and even the value of the wave function at the classical singularity is determined. In the isotropic case, direct symmetrization would lead to a breakdown of evolution, which thus provides an example for singular quantum evolution and demonstrates the non-triviality of continuing evolution: leading order coefficient would then be $V_{\mu-3\delta} - V_{\mu-5\delta} + V_{\mu+\delta} - V_{\mu-\delta}$, which vanishes if and only if $\mu = 2\delta$. Thus, in the backward evolution $\psi_{-2\delta}$ remains undetermined, just as ψ_0 is undetermined in the non-symmetric ordering. However, now $\psi_{-2\delta}$ would be needed to evolve further. Since it is not determined by initial data, one would need to prescribe this value, or else the evolution stops. There is thus a new region at negative μ, but evolution does not continue uniquely between the two sides. In such a case, even though curvature is bounded, the quantum system would be singular. A similar behavior happens in other orderings such as when triads are ordered to the left. Note that in the full theory as well one cannot order triads to the left since the constraint would otherwise not be densely defined [292].

The breakdown of the symmetric ordering in isotropic models is special and related to the fact that all directions degenerate. The breakdown does not happen for symmetric ordering in anisotropic or even inhomogeneous systems. One can avert it in isotropic cases by multiplying the constraint with $\mathrm{sign}(\hat{p})$ before symmetrizing, so that the additional factor of $\mathrm{sign}(\mu)$ leads to non-zero coefficients as in Equation (55).

This is the general scheme, which also applies in more complicated cases. First, the mechanism is independent of the precise form of matter since the Hamiltonian does not change the recurrence scheme. This holds true even for a non-minimally coupled scalar [94], even though one might suspect that the curvature coupling could also affect the highest-order terms of the difference equation. Similarly, the mechanism is robust under weakening of the symmetry. The prime example for general homogeneous behavior is given by the Kasner evolution of the Bianchi I model. Here, the approach to the singularity is anisotropic and given in such a way that two of the three diagonal metric components become zero while the third one diverges. This would lead to a different picture than described before, since the classical singularity then lies at the infinite boundary of metric or co-triad minisuperspace. Also, unlike the isotropic case, densities or curvature potentials are not necessarily bounded in general as functions on minisuperspace, and the classical dynamical approach is important. In densitized triad variables, however, we have a situation as before, since here all components approach zero, although at different rates. Now the classical singularity is in the interior of minisuperspace and one can study the evolution as before, again right through the classical singularity. Note that densitized triad variables were required for a background-independent quantization, and now independently for non-singular evolution.

Other homogeneous models are more complicated since for them Kasner motion takes place with a potential given by curvature components. Approximate Kasner epochs arise when the potential is negligible, intermitted by reflections at the potential walls where the direction of Kasner motion in the anisotropy plane changes. Still, since in each Kasner epoch the densitized triad components decrease, the classical singularity remains in the interior and is penetrated by the discrete quantum evolution.

One can use this for indications as to the general inhomogeneous behavior by making use of the BKL scenario. If this can be justified, in each spatial point the evolution of geometry is given by a homogeneous model. For the quantum formulation this indicates that, here also, classical singularities are removed. However, it is by no means clear whether the BKL scenario applies at the quantum level since even classically it is not generally established. If the scenario is not realized (or if some matter systems can change the local behavior), diverging p are possible and the behavior would qualitatively be very different. One has to study the inhomogeneous quantum evolution directly as done before for homogeneous cases. Note also that bounce models of non-singular evolution can typically not be straightforwardly combined with the BKL scenario because they avoid the asymptotic regime used in BKL constructions.

In the one-dimensional models described here classical singularities arise when E^x becomes zero. Since this is now a field, it depends on the point x on the spatial manifold where the slice hits the classical singularity. At each such place, midisuperspace opens up to a new region not reached by the classical evolution, where the sign of $E^x(x)$ changes and thus the local orientation of the triad. Again, the kinematics automatically provides us with these new regions just as needed, and quantum evolution continues. The scheme is realized much more non-trivially, and now even non-symmetric ordering is not allowed. This is a consequence of the fact that $k_e = 0$ for a single edge label does not imply that neighboring volume eigenvalues vanish. There is no obvious decoupling in a nonsingular manner, and it shows how less-symmetric situations put more stringent restrictions on the allowed dynamics. Still, the availability of other possibilities, perhaps with leading coefficients that can vanish and result in decoupling, needs to be analyzed. Most importantly, the symmetric version still leads to non-singular evolution even in those inhomogeneous cases that have local gravitational degrees of freedom [65].

Thus there is a general scheme for the removal of singularities: in the classical situation, one has singular boundaries of superspace which cannot be penetrated. Densitized triad variables then lead to new regions, given by a change in the orientation factor $\mathrm{sign}(\det(E))$, which, however, does not help classically since singularities remain as interior boundaries. For the quantum situation one has to look at the constraint equation and see whether or not it uniquely allows a wave function to continue to the other side (and does not require time parameters, even though they may be helpful if available). This usually depends on factor ordering and other choices that arise in the construction of constraint operators and play a role for the anomaly issue as well. Thus, one can fix ambiguities by selecting a nonsingular constraint if possible. However, the existence of nonsingular versions, as realized in a natural fashion in homogeneous models, is a highly non-trivial and by-no-means automatic property of the theory showing its overall consistency.

In inhomogeneous models the issue is more complicated. We have a situation where the theory, so far well defined, can be tested by trying to extend results to more general cases. It should also be noted that different models should not require different quantization choices unless symmetry itself is clearly responsible (as happens with the orientation factor in the symmetric ordering for an isotropic model, or when non-zero spin connection components receive covariant meaning in models), but that there should rather be a common scheme leading to non-singular behavior. This puts further strong conditions on the construction and is possible only if one knows how models and the full theory are related.

5.17 Initial/boundary value problems

> Manto: *"Ich harre, um mich kreist die Zeit."*
>
> (Manto: *"I stand still, around me circles time."*)
>
> Goethe
> Faust

In isotropic models the gravitational part of the constraint corresponds to an ordinary difference operator, which can be interpreted as generating evolution in internal time. Thus one needs to specify only initial conditions to solve the equation. The number of conditions is large since, first, the procedure to construct the constraint operator usually results in higher-order equations and, second, this equation relates values of a wave function ψ_μ defined on an uncountable set. (The number of solutions for non-equidistant difference equations as they arise from refinement models has not been studied in detail and remains poorly understood.) In general, one has to choose a function on a real interval unless further conditions are used.

This can be achieved, for instance, by using observables that can reduce the kinematical framework back to wave functions defined on a countable discrete lattice [302]. Similar restrictions can come from semiclassical properties or the physical inner product [243], all of which has not yet been studied in generality.

The situation in homogeneous models is similar, but now one has several gravitational degrees of freedom only one of which is interpreted as internal time. One has a partial difference equation for a wave function on a minisuperspace with boundary, and initial as well as boundary conditions are required [56]. Boundary conditions are imposed only at nonsingular parts of minisuperspace, such as $\mu = 0$ in LRS models (57). They must not be imposed at places of classical singularities, of course, where instead the evolution must continue just as it does at any regular part.

In inhomogeneous models, then, there are not only many independent kinematical variables but also many difference equations for only one wave function on midisuperspace. These difference equations are similar to those in homogeneous models, but they are coupled in complicated ways. Since one has several choices in the general construction of the constraint, there are different possibilities for the way difference equations arise and are coupled. Not all of them are expected to be consistent, i.e., in many cases some of the difference equations will not be compatible such that there would be no non-zero solution at all. This is related to the anomaly issue since the commutation behavior of difference operators is important for properties and the existence of common solutions.

The difference equations of loop quantum cosmology thus provide a general existence problem in analogy to the classical initial-value problem of general relativity. It plays a direct role in the singularity issue, which can be cast in the form of quantum hyperbolicity [71]: if a wave function on all of minisuperspace is completely determined by initial and boundary values, it can be evolved, in particular, through a classical singularity, which thus does not pose a boundary to quantum evolution. Here, special properties of difference as opposed to differential equations play an important role: "mantic" states such as $|0\rangle$ in isotropic models can occur, whose coefficient in a state drops out of the recurrence relation instead of causing its breakdown. This formulation of the singularity issue is different from the usual one in the classical theory, making use of geodesic completeness. But it is closely related to the alternative classical formulation of generalized hyperbolicity [129, 304, 305] according to which a spacetime is nonsingular if it gives rise to well-posed evolution for field theories. By avoiding the use of geodesics and directly using potentially physical field theories, such a formulation is more suitable to be compared to quantum theories such as loop quantum cosmology with its principle of quantum hyperbolicity.

So far, the evolution operator in inhomogeneous models has not been studied in detail, and solutions in this case remain poorly understood. Thus, information on the quantum hyperbolicity problem is far from complete. The difficulty of this issue can be illustrated by the expectations in spherical symmetry, in which there is only one classical physical degree of freedom. If this is to be reproduced for semiclassical solutions of the quantum constraint, there must be a subtle elimination of infinitely many kinematical degrees of freedom such that in the end only one physical degree of freedom remains. Thus, from the many parameters needed in general to specify a solution to a set of difference equations, only one can remain when compatibility relations between the coupled difference equations and semiclassicality conditions are taken into account.

How much this cancellation depends on semiclassicality and asymptotic infinity conditions remains to be seen. Some influence is to be expected since classical behavior should have a bearing on the correct reproduction of classical degrees of freedom. However, it may also turn out that the number of solutions to the quantum constraint is more sensitive to quantum effects. It is already known from isotropic models that the constraint equation can imply additional conditions for solutions beyond the higher-order difference equation, as we will discuss in Section 5.19. This usually arises at the location of classical singularities where the order of the difference equation can change. Since quantum behavior at classical singularities is important for all these issues, the number of solutions can be different from the classically-expected freedom, even when combined with possible semiclassical requirements far away from the singularity.

A further illustration of the importance of such conditions is provided by the Schwarzschild interior, an anisotropic model [14]. As observed in [123], conditions on the wave function arising at the classical singularity imply that any physical solution is symmetric under orientation reversal (which is not guaranteed by other properties of the theory). Since the orientation changes during singularity traversal in loop quantum cosmology, this implies that the states before and after the Schwarzschild singularity are identical to each other, just as it is expected for a solution to be matched to a static exterior geometry. When there is collapsing matter, such a symmetry is no longer expected and the anisotropic but homogeneous model used to describe the Schwarzschild interior can no longer be used. In such a situation one would have to use spherically-symmetric states, which have a more complicated behavior. These relations provide interesting indications for an overall consistent general behavior.

We will now first discuss requirements for semiclassical regimes, followed by more information on possibly-arising additional conditions for solutions given in Section 5.19.

5.18 Pre-classicality and boundedness

The high order of difference equations implies that there are in general many independent solutions, most of which are oscillating on small scales, i.e., when the labels change only slightly. One possibility to restrict the number of solutions then is to require suppressed or even absent oscillations on small scales [48]. Intuitively, this seems to be a prerequisite for semiclassical behavior and has therefore been called Pre-classicality. It can be motivated by the fact that a semiclassical solution should not be sensitive to small changes of, e.g., the volume by amounts of Planck size. However, even though the criterion sounds intuitively reasonable, there is so far not much justification through more physical arguments involving observables or measurement processes to extract information from wave functions. One possible mechanism is that group averaging the connection dependent constraint would have to result in almost constant physical states. The exponentiated constraint is not a precise translation operator because it is not linear in the connection and also depends on the triad and matter, and so states would certainly change on larger scales. In this way, Pre-classicality might be related to physical normalization. Overall, however, the status of Pre-classicality as a selection criterion is not final.

Moreover, Pre-classicality is not always consistent in all disjoint classical regimes or with other conditions. For instance, as discussed in the following section, there can be additional conditions on wave functions arising from the constraint equation at the classical singularity. Such conditions do not arise in classical regimes, but they nevertheless have implications for the behavior of wave functions there through the evolution equation [124, 122]. It may also not be possible to impose Pre-classicality in all disconnected classical regimes. If the evolution equation is locally stable – which is a basic criterion for constructing the constraint – choosing initial values in classical regimes, which do not have small-scale oscillations, guarantees that oscillations do not build up through evolution in a classical regime [79]. However, when the solution is extended through the quantum regime around a classical singularity, oscillations do arise and do not in general decay after a new supposedly-classical regime beyond the singularity is entered. It is thus not obvious that indeed a new semiclassical region forms, even if the quantum evolution for the wave function is nonsingular. On the other hand, evolution does continue to large volume and macroscopic regions, which is different from other scenarios, such as [179] where inhomogeneities have been quantized on a background.

A similar issue is the boundedness of solutions, which is also motivated intuitively by referring to the common-probability interpretation of quantum mechanics [174], but must be supported by an analysis of physical inner products. The issue arises, in particular, in classically forbidden regions where one expects exponentially growing and decaying solutions. If a classically forbidden region extends to infinite volume, as happens for models of re-collapsing universes, the probability interpretation would require that only the exponentially decaying solution is realized. As before, such a condition at large volume is in general not consistent in all asymptotic regions or with other conditions arising in quantum regimes. For a free, massless scalar as matter source one can compute the physical inner product with the result that physical solutions indeed decay beyond the collapse point [28].

Both issues, pre-classicality and boundedness, seem to be reasonable, but their physical significance has to be founded on properties of the physical inner product. They are rather straightforward to analyze in isotropic models without matter fields, where one is dealing with ordinary difference equations. However, other cases can be much more complicated such that conclusions drawn from isotropic models alone can be misleading. Moreover, numerical investigations have to be taken with care since, in particular for boundedness, an exponentially increasing contribution can easily arise from numerical errors and dominate the exact, potentially-bounded solution.

Thus, one needs analytical or at least semi-analytical techniques to deal with these issues. For pre-classicality one can advantageously use generating function techniques [124], if the difference equation is of a suitable form, e.g., has only coefficients with integer powers of the discrete parameter. The generating function $G(x) := \sum_n \psi_n x^n$ for a solution ψ_n on an equidistant lattice then solves a differential equation equivalent to the difference equation for ψ_n. If $G(x)$ is known, one can use its pole structure to get hints for the degree of oscillation in ψ_n. In particular, the behavior around $x = -1$ is of interest to rule out alternating behavior where ψ_n is of the form $\psi_n = (-1)^n \xi_n$ with $\xi_n > 0$ for all n (or at least all n larger than a certain value). At $x = -1$ we then have $G(-1) = \sum_n \xi_n$, which is less convergent than the value for a non-alternating solution $\psi_n = \xi_n$ resulting in $G(-1) = \sum_n (-1)^n \xi_n$. One can similarly find conditions for the pole structure to guarantee boundedness of ψ_n, but the power of the method depends on the form of the difference equation. Generating functions have been used in several cases for isotropic and anisotropic models [122, 143, 123]. More general techniques are available for the boundedness issue, and also for alternating behavior, by mapping the difference equation to a continued fraction which can be evaluated analytically or numerically [101]. One can then systematically find initial values for solutions that are guaranteed to be bounded.

5.19 Dynamical initial conditions

> *I am Aton when I am alone in the Nun, but I am Re when he appears, in the moment when he starts to govern what he has created.*
>
> Book of the Dead

The traditional subject of quantum cosmology is the imposition of initial conditions on the wave function of a universe in order to guarantee its uniqueness. In the Wheeler–DeWitt framework this is done at the singularity $a = 0$, sometimes combined with final conditions in the classical regime. One usually uses intuitive pictures as guidance, akin to Lemaitre's primitive atom whose decay is supposed to have created the world, Tryon's and Vilenkin's tunneling event from nothing, or the closure of spacetime into a Euclidean domain by Hartle and Hawking.

In the latter approaches, which have been formulated as initial conditions for solutions of the Wheeler–DeWitt equation [306, 176], the singularity is still present at $a = 0$, but reinterpreted as a meaningful physical event through the conditions. In particular, the wave function is still supported at the classical singularity, i.e., $\psi(0) \neq 0$, in contrast to DeWitt's original idea of requiring $\psi(0) = 0$ as a means to argue for the absence of singularities in quantum gravity [152]. DeWitt's initial condition is in fact, though most appealing conceptually, not feasible in general since it does not lead to a well-posed initial value formulation in more complicated models: the only solution would then vanish identically. Zeh tried to circumvent this problem, for instance by proposing an ad hoc Planck potential, which is noticeable only at the Planck scale and makes the initial problem well defined [131]. However, the problem remains that in general there is no satisfying origin of initial values.

In all these ideas, the usual picture in physics has been taken; that there are dynamical laws describing the general behavior of a physical system, and independent initial or boundary conditions to select a particular situation. This is reasonable since one can usually prepare a system, correspondent to chosen initial and boundary values, and then study its behavior as determined by the dynamical laws. For cosmology, however, this is not appropriate since there is no way to prepare the universe.

At this point, loop quantum cosmology opens up a new possibility, in which the dynamical laws and initial conditions can be part of the same entity [48, 112, 57]. This is a specialty of difference equations, whose order can change locally, in contrast to differential equations. Mathematically, such a difference equation would be called singular, since its leading-order coefficients can become zero. However, physically we have already seen that the behavior is non-singular, since the evolution does not break down.

The difference equation follows from the constraint equation, which is the primary object in canonical quantum gravity. As discussed before, it is usually of high order in classical regimes, where the number of solutions can be restricted, e.g., by pre-classicality. But this, at most, brings us to the number of solutions that we have for the Wheeler–DeWitt equation, such that one needs additional conditions as in this approach. The new aspect is that this can follow from the constraint equation itself: since the order of the difference equation can become smaller at the classical singularity, there are less solutions than expected from the semiclassical behavior. In the simplest models, this is just enough to result in a unique solution up to norm, as appropriate for a wave function describing a universe. In those cases, the dynamical initial conditions are comparable to DeWitt's initial condition, albeit in a manner that is well posed, even in some cases where DeWitt's condition is not [89].

In general, the issue is not clear but should be seen as a new option presented by the discrete formulation of loop quantum cosmology. Since there can be many conditions to be imposed on wave functions in different regimes, one must determine for each model whether or not suitable non-zero solutions remain. In fact, some first investigations indicate that different requirements taken together can be very restrictive [122], which seems to relate well with the non-separability of the kinematical Hilbert space [143]. So far, only homogeneous models have been investigated in detail, but the mechanism of decoupling is known not to be realized in an identical manner in inhomogeneous models.

Inhomogeneous models can qualitatively add new ingredients to the issue of initial conditions due to the fact that there are many coupled difference equations. There can then be consistency conditions for solutions to the combined system, which can strongly restrict the number of independent solutions. This may be welcome, e.g., in spherical symmetry, where a single physical parameter remains, but the restriction can easily become too strong, with a number of solutions even below the classically expected one. Since the consistency between difference equations is related to the anomaly issue, there may be an important role played by quantum anomalies. While classically anomalies should be absent, the quantum situation can be different, since it also takes the behavior at the classical singularity into account and is supposed to describe the whole universe. Anomalies can then be precisely what one needs in order to have a unique wave function of a universe even in inhomogeneous cases where initially there is much more freedom. This does not mean that anomalies are simply ignored or taken lightly, since it is difficult to arrange having the right balance between many solutions and no nonzero solutions at all. However, quantum cosmology suggests that it is worthwhile to have a less restricted, unconventional view on the anomaly issue.

5.20 Numerical and mathematical quantum cosmology

The analysis of difference equations as they arise in loop quantum cosmology can benefit considerably from the application of numerical techniques. Compared to a numerical study of differential equations, the typical problems to be faced take a different form. One does not need to discretize difference equations before implementing a numerical code, which eliminates choices involved in this step but also removes some of the freedom, which is often exploited to devise powerful codes. In particular, stability issues take a different form in loop quantum cosmology. The only freedom one has in the "discretization" are quantization choices, which affect the end result of a difference equation, but this is much more indirect to apply. Nevertheless, such studies can, for the same reason, provide powerful feedback on how the dynamics of quantum gravity should be formulated [79].

Isotropic difference equations for the gravitational degree of freedom alone are straightforward to implement, but adding a second degree of freedom already makes some of the questions quite involved. This second degree of freedom might be a conventionally quantized scalar, in which case the equation may be of mixed difference/differential type, or an anisotropy parameter. The first non-trivial numerical analysis was done for an isotropic model, but for a solution of the gauge evolution of non-physical states generated by the Hamiltonian constraint [103]. Thus, the second "degree of freedom" here was coordinate time. A numerical analysis with a scalar field as internal time was done in [280]. Numerical investigations for the first models with two true gravitational degrees of freedom were performed in the context of anisotropic and especially black hole interior models [130, 123], which in combination with analytical tools have provided valuable insights into the stability issue [250]. Stability, in this case, requires non-trivial refinement models, which necessarily lead to non-equidistant difference equations [75]. This again poses new numerical issues, on which there has recently been some progress [262]. Variational and other methods have been suggested [275, 274], but not yet developed into a systematic numerical tool.

A scalar as a second degree of freedom in an isotropic model does not lead to severe stability issues. For a free and massless scalar, moreover, one can parameterize the model with the scalar as internal time and solve the evolution it generates. There is a further advantage because one can easily derive the physical inner product, and then numerically study physical states [26, 28]. This has provided the first geometrical pictures of a bouncing wave function [25]. The same model is discussed from the perspective of computational physics in [211].

Here also, long-term evolution can be used to analyze refinement models [27], although the emphasis on isotropic models avoids many issues related to potentially non-equidistant difference equations. Numerical results for isotropic free-scalar models also indicate that they are rather special, because wave functions do not appear to spread or deform much, even during long-term evolution. This suggests that there is a hidden solvability structure in such models, which was indeed found in [70]. As described in Section 6, the solvability provides new solution techniques as well as generalizations to non-solvable models by the derivation of effective equations in perturbation theory. Unless numerical tools can be generalized considerably beyond isotropic free-scalar models, effective techniques seem much more feasible to analyze, and less ambiguous to interpret, than results from this line of numerical work.

The derivation and analysis of such effective systems has, by the existence of an exactly solvable model, led to a clean mathematical analysis of dynamical coherent states suitable for quantum cosmology. In particular, the role of squeezed states has been highlighted [69, 74]. Further mathematical issues show up in possible extensions of these results to more realistic models. Independently, some numerical studies of loop quantum cosmology have suggested a detailed analysis of self-adjointness properties of Hamiltonian constraint operators used. In some cases, essential self-adjointness can strictly be proven [286, 285, 197], but there are others where the constraint is known not to be essentially self-adjoint. Possible implications of the choice of a self-adjoint extension are under study. Unfortunately, however, the theorems used so far to conclude essential self-adjointness only apply to a specific factor ordering of the constraint, which splits the two sine factors of $\sin^2 \delta c$ in Equation (52) arising from the holonomy $h_I h_J h_I^{-1} h_J^{-1}$ around a square loop evaluated in an isotropic connection; see Section 5.4. This splitting with both factors sandwiching the commutator $h_K[h_K^{-1}, \hat{V}]$ could not be done under general circumstances, where one only has the complete h_α along some loop α as a single factor in the constraint. Thus the e mathematical techniques used need to be generalized.

5.21 Summary

There is a general construction of a loop representation in the full theory and its models, which is characterized by compactified connection spaces and discrete triad operators. Strong simplifications of some technical and conceptual steps occur in diverse models. Such a general construction allows a view not only in the simplest case, isotropy, but in essentially all representative systems for gravity.

Most important is the dynamics, which in the models discussed here can be formulated by a difference equation on superspace. A general scheme for a unique extension of wave functions through classical singularities is realized, such that the quantum theory is non-singular. This general argument, which has been verified in many models, is quite powerful since it does not require detailed knowledge of, or assumptions about, matter. It is independent of the availability of a global internal time, and so the problem of time does not present an obstacle. Moreover, a complicated discussion of quantum observables can be avoided since once it is known that a wave function can be continued uniquely, one can extract relational information at both sides of the classical singularity. (If observables would distinguish both sides with their opposite orientations, they would strongly break parity even on large scales in contradiction with classical gravity.) Similarly, information on the physical inner product is not required since there is a general statement for all solutions of the constraint equation. The uniqueness of an extension through the classical singularity thus remains, even if some solutions have to be excluded from physical Hilbert space or factored out if they have zero norm.

This is far from saying that observables or the physical inner product are irrelevant for an understanding of dynamical processes. Such constructions can, fortunately, be avoided for a general statement of non-singular evolution in a wide class of models. For details of the transition and to get information on the precise form of spacetime at the other side of classical singularities, however, all those objects are necessary and conceptual problems in their context have to be understood.

So far, the transition has often been visualized by intuitive pictures such as a collapsing universe turning inside out when the orientation is reversed. An hourglass is a good example of the importance of discrete quantum geometry close to the classical singularity and the emergence of continuous geometry on large scales: away from the bottleneck of the hourglass, its sand seems to be sinking down almost continuously. Directly at the bottleneck with its small circumference, however, one can see that time measured by the hourglass proceeds in discrete steps – one grain at a time.

Two issues remain: one would like to derive more geometrical or intuitive pictures of the non-singular behavior, such as those discussed in Section 4, but on a firmer basis. This can be done by effective equations as discussed in Section 6. Then there is the question of how models are related to the full theory and to what extent they are characteristic of full quantum geometry, which is the topic of Section 7.

6 Effective Theory

Even in isotropic models, difference equations of states can be difficult to analyze. And even if one finds solutions, analytically or numerically, one still has to face conceptual problems of interpreting the wave function correctly. In quantum physics there is a powerful tool, effective equations, which allows one to include quantum effects by correction terms in equations of the classical type. Thus, in quantum mechanics one would be dealing with effective equations, which are ordinary differential rather than partial differential equations. Moreover, the wave function would only appear indirectly and one solves equations for classical type variables such as expectation values with an immediate physical interpretation. Still, in some regimes quantum effects can be captured reliably by correction terms in the effective equations. Effective equations can thus be seen as a systematic approximation scheme to the partial differential equations of quantum mechanics.

Quantum cosmology is facing the problems of quantum mechanics, some of which in an even more severe form because one is by definition dealing with a closed system without outside observers. It also brings its own special difficulties, such as the problem of time. Effective equations can thus be even more valuable here than in other quantum systems. In fact, effective theories for quantum cosmology can be and have been derived and already provided insights, especially for loop quantum cosmology. These techniques and some of the results are described in this section. As we will see, some of the special problems of quantum gravity, such as the physical inner product and anomaly issues, are in fact much easier to deal with at an effective level compared to the underlying quantum theory, in terms of its operators and states. In addition to conceptual problems, phenomenological problems are addressed because effective equations provide the justification for the phenomenological correction terms discussed in Section 4. But they will also show that there are new corrections not discussed before, which have to be included for a complete analysis. Effective equations thus provide a means to test the self-consistency of approximations.

6.1 Solvable systems and perturbation theory

Quantum dynamics is given through a Hamiltonian operator $\hat{H}$, which determines the Schrödinger flow $i\hbar\dot{\psi} = \hat{H}\psi$, or alternatively Heisenberg equations of motion $\dot{\hat{O}} = -i\hbar^{-1}[\hat{O},\hat{H}]$ for time-dependent operators. Independent of the representation, expectation values obey the equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{O}\rangle = \frac{\langle[\hat{O},\hat{H}]\rangle}{i\hbar}\,. \tag{72}$$

For basic operators, such as $\hat{q}$ and $\hat{p}$ in quantum mechanics, we have a system

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{q}\rangle = \frac{\langle[\hat{q},\hat{H}]\rangle}{i\hbar} \quad , \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = \frac{\langle[\hat{p},\hat{H}]\rangle}{i\hbar} \tag{73}$$

of coupled equations, which, as in the Ehrenfest theorem, can be compared with the classical equations for q and p. However, the equations (73) in general do not form a closed set unless the commutators $[\hat{q},\hat{H}]$ and $[\hat{p},\hat{H}]$ are linear in the basic operators $\hat{q}$ and $\hat{p}$, such that only expectation values appear on the right-hand side of Equations (73). Otherwise, one has terms of the form $\langle\hat{q}^n\hat{p}^m\rangle$ with $n+m>1$, which, in quantum mechanics, are independent of the expectation values $\langle\hat{q}\rangle$ and $\langle\hat{p}\rangle$. There is no closed set of equations unless one includes the dynamics of all the moments of a state related to the additional terms $\langle\hat{q}^n\hat{p}^m\rangle$. A more practical formulation refers to the infinite-dimensional quantum phase space parameterized by expectation values together with the quantum variables $G^{a,n}$ of Equation (56). Poisson relations between all these variables follow from expectation values of commutators, and are available in general form [105, 282]. The flow on this quantum phase space is then simply given by the quantum Hamiltonian defined as the expectation value $H_Q = \langle\hat{H}\rangle$ of the Hamiltonian, interpreted as a function of the quantum variables, which parameterize the state used in the expectation value. Also here, in general, coupling terms between expectation values and quantum variables arise in H_Q, which then couple the Hamiltonian equations of motion obtained from H_Q for the expectation values and all the quantum variables. But these would be infinitely many coupled ordinary differential equations, which usually is much more complicated to solve than the single partial Schrödinger equation.

Physically, this means that quantum mechanics is described by a wave function, where all the moments, such as fluctuations and deformations from a Gaussian, play a role in the dynamical evolution of expectation values. These quantum variables evolve, and in general couple the expectation values due to quantum backreaction. This quantum backreaction is the reason for quantum corrections to classical dynamics, which is often usefully summarized in effective equations. Such equations, which have the classical form but are amended by quantum corrections, are much easier to solve and more intuitive to understand than the full quantum equations. But they have to be derived from the quantum system in the first place, which does require an analysis of the infinitely-many coupled equations for all moments.

Fortunately, this can often be done using approximation schemes, such as semiclassical expansions and perturbation theory. For this, one needs a treatable starting point as the zeroth order of the perturbation theory, a solvable model, whose equations of motion for moments are automatically decoupled from those for expectation values. Such models are the linear ones, where commutators $[\cdot, \hat{H}]$ between the basic operators and the Hamiltonian are linear in the basic operators. For a canonical algebra of basic operators such as $[\hat{q}, \hat{p}] = i\hbar$, the Hamiltonian must be quadratic, e.g., be that of the harmonic oscillator. Then, the quantum equations of motion for $\hat{q}$ and $\hat{p}$ decouple from the moments and form a finite set, which can be easily solved. The harmonic oscillator is not the only quadratic Hamiltonian, but it is special because it allows (coherent state) solutions, whose higher moments are all constant. (This corresponds to the horizontal sections of the quantum phase space mentioned in Section 5.6.2.)

This explains the special role of the harmonic oscillator (or massive free field theories) in perturbation theory: any linear system can be used as zeroth order in a semiclassical perturbation expansion for models, which add interactions, i.e., non-quadratic terms, to the Hamiltonian and thus coupling terms between expectation values and quantum variables. In general, this results in higher-dimensional effective systems, where some of the quantum variables, but only finite ones, may remain as independent variables. If one perturbs around the harmonic oscillator, on the other hand, the fact that it allows solutions (especially the ground state) with constant quantum variables, allows an additional approximation, using adiabatic behavior of the quantum variables. In this case, one can even solve for the remaining quantum variables in terms of the classical variables, which provides explicit effective potentials and other corrections without having to refer to quantum degrees of freedom. In this way, for instance, one can derive the low-energy effective action well known from particle physics [105, 282]. This behavior, however, is not general because not all linear systems allow the adiabaticity assumption. For instance, a free particle, whose Hamiltonian is also quadratic, violates the adiabaticity assumption. Correspondingly, quantum terms in the low-energy effective action diverge when the frequency of the harmonic oscillator approaches zero, a fact that is known as infrared divergence in quantum field theory. Higher dimensional effective systems, where some quantum variables remain as independent degrees of freedom, still exist. Similar techniques are applied to cosmological structure formation in [104], with possible applications to non-Gaussianities.

6.2 Effective constraints

In Section 6.1 we describe how effective equations for an unconstrained system are obtained. Gravity as a fully constrained system requires an extension of the methods to dynamics provided by a Hamiltonian constraint $\hat{C}$ rather than a Hamiltonian $\hat{H}$. In this case, the expectation value

$C_Q = \langle \hat{C} \rangle$, again interpreted as a function on the infinite dimensional quantum phase space, plays a role similar to H_Q. Thus, the main constraint equation of the effective theory is obtained through expectation values of the constraint operator, which will play a role in applications to loop quantum cosmology. However, several new features arise for constrained systems.

First, it is not sufficient to consider a single effective constraint for every constraint operator. This can easily be seen because one (first class) constraint removes one pair of canonical variables. The quantum phase space, however, has infinitely many quantum variables for each classical canonical pair. If only one effective constraint were imposed, the quantum variables of the constrained pair would remain in the system and possibly couple to other variables, although they correspond to gauge degrees of freedom. Additional effective constraints are easy to find: if the quantum phase space is to be restricted to physical states, then not only $\langle \hat{C} \rangle$ but also $\langle \hat{C}^n \rangle$ and even expressions such as $\langle \hat{O}\hat{C}^n \rangle$ for arbitrary powers $n > 0$ and operators $\hat{O}$ must vanish. This provides infinitely many constraints on the quantum phase space, from which one should select a complete subset. Doing so can depend on the precise form of the constraint and may be difficult in specific cases, but it has been shown to give the correct reduction in examples.

Secondly, for constraints, we have to keep in mind the anomaly issue. If one has several constraint operators, which are first class, then the quantum constraints obtained as their expectation values are also first class. Moreover, one can define complete sets of higher-power constraints, which preserve the first-class nature. Thus, the whole system of infinitely many quantum constraints is consistent. However, this does not automatically extend to the effective constraints obtained after truncating the infinitely many quantum variables. For the truncated, effective constraints one still has to make sure that no anomalies arise to the order of the truncation. Moreover, in complicated theories such as loop quantum gravity it is not often clear if the original set of constraint operators was first class. In such a case one can still proceed to compute effective constraints, since potential inconsistencies due to anomalies would only arise when one tries to solve them. After having computed effective constraints, one can then analyze the anomaly issue at this phase space stage, which is much easier than looking at the full anomaly problem for the constraint operators. One can then consistently define effective theories and see whether anomaly freedom allows non-trivial quantum corrections of a certain type. By proceeding to higher orders of the truncation, tighter and tighter conditions will be obtained in approaching the non-truncated quantum theory. (See Section 6.5.4 for applications.)

The third difference is that we now have to deal with the physical inner-product issue. Since the original constraints are defined on the kinematical Hilbert space, which is used to define the unconstrained quantum phase space, solving the effective constraints could change the phase-space structure. This is most easily seen for uncertainty relations, which provide inequalities for the second-order quantum variables $G^{a,n}$ and for canonical variables take the form

$$G^{0,2}G^{2,2} - (G^{1,2})^2 \geq \frac{\hbar^2}{4} \,. \tag{74}$$

Some of the effective constraints will constrain the quantum variables and could violate the original uncertainty relations, corresponding to the fact that the physical inner product would define a new Hilbert space and thus reduced quantum phase space structure. Alternatively, it is often more convenient to respect uncertainty relations, but allow complex solutions to the quantum constraints. By definition, quantum variables refer to expectation values of totally symmetric operators, which should be real. For a constrained system, however, this would refer to the kinematical Hilbert space structure. Violations of kinematical reality then indicate that the physical Hilbert space structure differs from the kinematical one. In fact, one can ensure the physical inner product by requiring that all quantum variables left after solving the quantum constraints are real. This has been shown to provide the correct results in examples, and is much easier to implement than finding an explicit inner product for states in a Hilbert space representation.

Thus, there are promising prospects for the usefulness of effective techniques in quantum gravity, which can even address anomaly and physical inner-product issues.

6.3 Isotropic cosmology

The use of $\langle\hat{C}\rangle$ for effective constraints explains why loop cosmology receives corrections from quantizations of the inverse volume and higher power corrections from holonomies. Such corrections must be present since the corresponding quantizations are crucial features of the full theory, and they have given rise to many phenomenological effects. (The precise form of corrections depends on the suitable semiclassical states used, while terms in phenomenological equations using effective densities, as well as higher powers of connection components, have been read off from expressions in eigenstates of triads or holonomies. Qualitative features are insensitive to the difference, and so simply reading off terms is good enough for phenomenology.) But for a reliable analysis one must to derive a complete set of quantum corrections to any given order, which the phenomenological corrections described in Section 4 cannot provide because they ignore quantum backreaction, the main source of corrections in genuine quantum systems. A systematic analysis of possible coupling terms between expectation values and quantum variables is required.

Our cosmology, however, is not close to a harmonic oscillator, which makes this solvable system unsuitable as zeroth order for a perturbative analysis. There is, however, a solvable system available for quantum cosmology: a spatially-flat isotropic model sourced by a free scalar [70]. The Friedmann equation, written in isotropic Ashtekar variables, is

$$c^2\sqrt{|p|} = \frac{4\pi G}{3}\frac{p_\phi^2}{|p|^{3/2}}\,. \tag{75}$$

This is certainly a constraint, and so we could use the framework of effective constraints. In this form, however, the system would not be recognized as solvable because the constraint is obviously not quadratic in the canonical variables. On the other hand, in this case, it is easy to parameterize the system by choosing the scalar ϕ as internal time. Then, the solution

$$|p_\phi| = \frac{3}{4\pi G}|pc| = H(p,c) \tag{76}$$

of (75) provides an ordinary Hamiltonian $H(p,c)$ for ϕ-evolution, which, except for the absolute value, is quadratic. The absolute value can in fact be shown to be irrelevant for the most interesting aspects of these kinds of cosmologies [69], such that we obtain a solvable system for quantum cosmology.

More remarkably, this solvability behavior even extends to loop quantum cosmology. In this case, there is no operator for c and thus one has to refer to non-canonical variables involving holonomies or the exponentials e^{ic}. For this reason, the Hamiltonian operator as constructed in Section 5.4 receives higher-order corrections and takes the form $\hat{H} = \widehat{p\sin c}$ in a certain factor ordering. Since this is no longer quadratic in canonical variables and we are forced to use a non-canonical basic operator algebra, it seems difficult to relate this to the solvable free scalar cosmology. However, there is a change of basic variables, which provides an exact solvable model even for loop quantum cosmology: using $\hat{p}$ and $\hat{J} := \hat{p}\exp(ic)$ (in this ordering) as basic operators, we obtain a closed algebra of basic variables together with the Hamiltonian operator $\hat{H} = -\frac{1}{2}i(\hat{J}-\hat{J}^\dagger)$. This provides a solvable model for loop quantum cosmology as the starting point for a systematic derivation of effective equations.

While we keep calling the geometrical variable p, one should note that the solvable model is insensitive to the precise form of refinement used in the underlying quantization. Instead of starting with the canonical pair (c,p), one can use

$$v := \frac{p^{1-x}}{1-x} \quad \text{and} \quad P := p^x c, \tag{77}$$

which is also canonical. For $-1/2 < x < 0$ we obtain precisely the refinement models discussed in Sections 5.5 and 6.4 with $\delta(p) = p^x$. For any x, we are led to the same algebra of quantum operators between $\hat{v}$, $\hat{J} = \hat{v}\exp(iP)$ and a linear Hamiltonian $\hat{H} = -\frac{1}{2}i(\hat{J} - \hat{J}^\dagger)$ [69]. Only the geometrical interpretation of the variables depends on x.

This model also provides an instructive example for the role of physical inner-product issues in effective theory. By our definition of $\hat{J}$, we will have to deal with complex-valued expectation values of our basic operators, in particular $\langle\hat{J}\rangle$. After solving the effective equations, we have to impose reality conditions, which, due to the form of $\hat{J}$, are not linear but derived from the quadratic relation $\hat{J}\hat{J}^\dagger = \hat{p}^2$. Taking an expectation value of this relation provides the reality condition to be imposed, which not only involves expectation values but also fluctuations. Thus, fluctuations can in principle play a significant role for admissible solutions, but this does not happen for initially semiclassical states. Physical solutions for expectation values and higher moments can then be found more conveniently than it would be for states in a Hilbert-space representation.

Thanks to the solvability of this model it is clear that it does not receive quantum corrections from backreaction. Thus, it is strictly justified in this model to use higher-power corrections as they are implemented by $\sin c$. But inverse volume corrections have been neglected by construction, since they would alter the Hamiltonian and destroy the solvability. In a complete treatment, such corrections would have to arise, too, and with them quantum backreaction would play a role in the absence of solvability. Nevertheless, for many applications, one can argue that the latter types of corrections are small in an isotropic model because one usually requires a large matter content and thus large p_ϕ, which enhances higher-power corrections. However, the situation is not fully clarified since the original versions, where the magnitudes of higher power and inverse volume corrections were compared numerically [26, 27, 28], were based on formulations of isotropic loop quantum cosmology, where inverse volume corrections are artificially suppressed due to the form of the symmetry reduction [75]. Taking this into account makes inverse volume corrections important for a larger parameter range. They are also much more prominent in inhomogeneous models.

Independent of this question, quantum backreaction inevitably results in the presence of matter interactions, anisotropies or inhomogeneities. In those cases, taking higher-power corrections, as in the free isotropic model, is not as reliable, and a detailed analysis is required, which so far has been provided only for a perturbative treatment of scalar potentials [87]. As anticipated, the resulting effective equations do not seem to allow an adiabatic approximation since quantum variables in the underlying solvable models are not constant. One thus has to deal with higher-dimensional effective systems, where some of the quantum variables remain as independent variables. Effective equations have been derived to first order in the perturbative potential and in a semiclassical expansion, but are rather involved and have not been analyzed much yet.

6.4 Inhomogeneity

Inhomogeneities can only be treated in a field-theory context, which requires infinitely many classical and quantum variables. The discreteness of loop quantum gravity might help in avoiding some of the field theory subtleties, since finite regions contain only finitely many variables. But there are still many of them, and the dynamical equations are rather involved. At present, it is only possible to include inhomogeneities in the sense of classical cosmological perturbation theory around isotropic models, where the isotropic background for the perturbations is introduced by selecting specific states within the background-independent quantum theory [66].

Since, even for isotropic models, complete effective equations have been derived only in rare cases so far, it will take longer to obtain complete effective equations for inhomogeneities. Nevertheless, the corrections can be derived systematically, and several of the simpler terms have already been obtained along the lines of [86]. Of advantage in this perturbative setting is the fact that, to linear order in inhomogeneities, one can split the perturbations in different modes (scalar, vector and tensor) and compute their corrections separately. For each mode, gauge invariant variables can be determined. This is discussed for scalar modes in [84, 92], for vector modes in [90] and for tensor modes in [91]. Such a procedure would not be available at higher orders, where cosmological observables can be computed in a canonical scheme [157, 156], but are difficult to introduce into a loop quantization.

Once effective equations for inhomogeneities have been obtained, valuable insights can be derived for fundamental, as well as phenomenological, questions. As already mentioned, effective constraints allow a simpler discussion of anomalies than the full quantum theory provides. Anomalies are a pressing issue in the presence of inhomogeneities since the constraint algebra is quite non-trivial. By analyzing whether anomaly freedom is possible in the presence of quantum corrections, one can get hints as to whether such quantizations can be anomaly free in a full setting. This usually leads to additional conditions on the corrections, by which one can reduce quantization ambiguities. Since closed equations of motion for gauge invariant perturbations are possible only in the absence of anomalies, this issue also has direct implications for phenomenology. Anomaly-free effective constraints and the equations of motion they generate can be formulated in terms of gauge invariant quantities only, where gauge invariance refers to gauge transformations generated by the effective constraints including corrections. In this way, a complete analysis can be performed and evaluated for cosmological effects.

Effective equations for inhomogeneous models also provide the means to analyze refinements of the underlying discreteness as they are suggested by the full Hamiltonian constraint operators. In this context, inhomogeneous considerations help to elucidate the role of certain auxiliary structures in homogeneous models, which have often led to a considerable amount of confusion. The basic objects of inhomogeneous states are edge holonomies of the form $\exp(i\ell_0\tilde{A})$ where ℓ_0 is the coordinate length of the edge and $\tilde{A}$ is some integrated connection component. (This may not directly be a component of A_a^i due to the path ordering involved in non-Abelian holonomies. Nevertheless, we can think of matrix elements of holonomies as of this form for the present purpose.) Similarly, basic fluxes are given by surfaces transversal to a single edge in the graph. These are the elementary objects on which constructions of inhomogeneous operators are based, in contrast to homogeneous models, where only the total space or a chosen box of size V_0, as in Section 4.2, is available to define edges for holonomies and surfaces for fluxes. Such a box is one of the auxiliary structures appearing in the definition of homogeneous models since there is no underlying graph to relate these objects to a state.

If a graph is being refined during evolution (in volume as internal time, say), the parameter ℓ_0 can be thought of as being non-constant, but rather a function of volume. Note that the whole expression of a holonomy is coordinate-independent since the product $\ell_0\tilde{A}$ comes from a scalar quantity. The refinement can thus also be formulated in coordinate independent terms. For instance, if we are close to an isotropic configuration, we can, as in Equation (22), introduce the isotropic connection component $c = V_0^{1/3}\tilde{A}$ with coordinate size V_0 of the above-mentioned box. Isotropic holonomies thus take the form $\exp(i\ell_0 V_0^{-1/3}c)$, where, for a nearly-regular graph with respect to the background geometry, $\ell_0/V_0^{1/3} =: \mathcal{N}^{-1/3}$ is the inverse cubic root of the number of vertices within the box. For a refining model, $\mathcal{N}$ increases with volume. For instance, if $\mathcal{N} \propto V$ with the total geometrical volume $V = |p|^{3/2}$ we have holonomies of the form $\exp(i\delta(p)c)$ with $\delta(p) \propto 1/\sqrt{|p|}$. This agrees with the suggestion of [27], or $x = -1/2$ in the notation of Section 5.5 [66], but is recognized here only as one special case of possible refinements. Moreover, one can easily convince oneself that a vertex number proportional to volume is not allowed by the dynamics of loop quantum gravity: this would require the Hamiltonian constraint to create only new vertices but not change the spin of edges. The other limiting case, where only spins change but no new vertices are created, corresponds to the non-refining model, where $\delta(p) = \text{const}$. A realistic refinement must therefore lie between those behaviors, i.e., $\delta(p) \propto |p|^x$ with $0 < x < -1/2$, if it follows a power law.

One can also see that V_0 appears only when the exactly isotropic model is introduced (possibly as a background for perturbations), but not in inhomogeneous models. Basic corrections are thus independent of V_0 and the chosen box. They refer rather to sizes of the elementary discrete variables: local edge holonomies and fluxes. This characterization is independent of any auxiliary structures but directly refers to properties of the underlying state. One should certainly expect this, because it is the quantum state, which determines the quantum geometry and its corresponding corrections to classical behavior.

6.5 Applications

Effective equations in the precise sense have already provided several applications to physical as well as conceptual questions of wider interest in quantum gravity.

6.5.1 Bounces

From the linear Hamiltonian $\hat{H} = -\frac{1}{2}i(\hat{J} - \hat{J}^\dagger)$ of Section 6.3 one obtains equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}\phi}\langle\hat{p}\rangle = -\frac{1}{2}(\langle\hat{J}\rangle + \langle\hat{J}^\dagger\rangle) \quad , \quad \frac{\mathrm{d}}{\mathrm{d}\phi}\langle\hat{J}\rangle = -\frac{1}{2}(\langle\hat{p}\rangle + \hbar) = \frac{\mathrm{d}}{\mathrm{d}\phi}\langle\hat{J}^\dagger\rangle\,. \tag{78}$$

(Again, we can replace p by v in Equation (77) and thus work with any refinement model in the same way.) They decouple from fluctuations or higher moments thanks to the solvability of the model. Solutions for the partially complex variables are subject to the reality condition

$$|\langle\hat{J}\rangle|^2 - (\langle\hat{p}\rangle + \tfrac{1}{2}\hbar)^2 = G^{pp} - G^{J\bar{J}} + \frac{1}{4}\hbar^2, \tag{79}$$

which follows from the identity $\hat{J}\hat{J}^\dagger = \hat{p}^2$ after taking expectation values and reformulating it in terms of expectation values p and J and their fluctuations. The general solution satisfying the reality condition (and assuming a state being semiclassical at least once) is [69]

$$\langle\hat{p}\rangle(\phi) = \langle\hat{H}\rangle\cosh(\phi - \delta) - \hbar \quad , \quad \langle\hat{J}\rangle(\phi) = -\langle\hat{H}\rangle(\sinh(\phi - \delta) - i), \tag{80}$$

where δ is a constant of integration. The solution for p obviously bounces, confirming the numerical results of [26].

For such a solvable model one can determine many more properties in detail, such as the behavior of fluctuations through the bounce and the role of coherent states. But the solvability of the model also reveals its very special nature, and, as well, that of all related numerical results, which are available so far. Initially, it came as a surprise that those numerical investigations were showing a nearly smooth bounce, with hardly any quantum effects deforming the wave packet or even leading to significant spreading. As quantum systems go, this is certainly not the expected behavior. Relating those models to a solvable one, where, as in the harmonic oscillator, moments only couple weakly or not at all to expectation values, demonstrates that the results are, after all, consistent with general expectations.

On the other hand, these models by themselves cannot be taken as an indication of the general behavior. If a matter potential is included, or anisotropies or inhomogeneities are taken care of, there will be quantum backreaction, as in typical quantum systems. States spread and deform during evolution, and it is no longer guaranteed that a state starting out semiclassically at large volume will remain so when it approaches the classical singularity. While the underlying difference equation is non-singular independent of quantum backreaction, the geometrical picture of non-singular behavior may well deviate strongly from a smooth bounce when the state is no longer semiclassical on small scales. (Note that phenomenological equations including higher powers of the connection, which are sometimes taken as indications for bounces, are themselves also subject to severe additional corrections in models with quantum backreaction.)

Moreover, even in these models one makes use of the large size of matter in the form of a large $\langle \hat{H} \rangle$. For smaller values even semiclassical states can enter the small-volume regime much more deeply, which then would require other corrections, such as those from effective densities. Assuming a large $\langle \hat{H} \rangle$ for the dynamics of local geometrical variables would no longer be justified in an inhomogeneous context, in addition to the then unavoidable quantum backreaction. Currently, robust demonstrations of bounces in loop quantum cosmology only refer to cases where quantum backreaction can safely be ignored, which are hardly realistic ones. Work on extending those results and on understanding the more general picture of non-singular quantum evolution is currently in progress; see also [110] for a discussion of the generality of present bounce results.

6.5.2 Before the Big Bang

The model of Section 6.3 for loop quantum cosmology allows precise results about the behavior of dynamical coherent states when they evolve through the point of the classical singularity. Not only can expectation values for volume and curvature describing the bounce be computed, but also fluctuations and higher moments of the state. Thus, one can see how a state evolves and whether the regime around the bounce has any implications. One can also analyze the full range of parameters determining such states in general, and thus address questions about how general certain properties, such as the approach to semiclassicality, are.

Of particular interest in the context of coherent states are fluctuations, which for the harmonic oscillator would remain constant. The system relevant for cosmology, however, is different and here fluctuations cannot be constant. Nevertheless, dynamical coherent states for the Wheeler–DeWitt model or the loop quantized model demonstrate that the ratios $(\Delta p)/p$ and $(\Delta c)/c$ remain constant for any part of the universe before or after the bounce. This implies that fluctuations can be huge because the solvable model has an unbounded p, but fluctuations relative to p stay small if they are small in a semiclassical initial state.

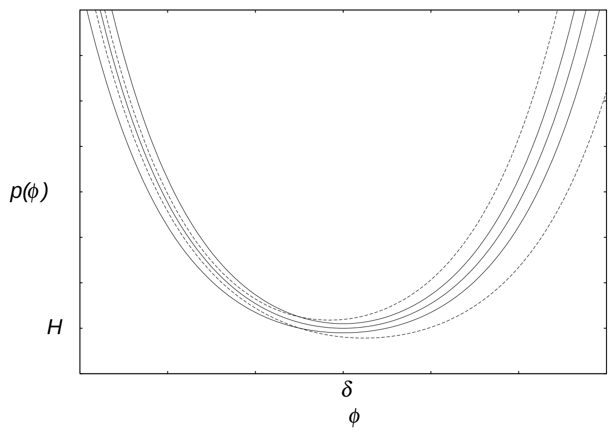

Figure 10: Internal time evolution for expectation values and spread of two bouncing states, one, which is unsqueezed (solid lines), and one, which is being squeezed (dashed).

This is not true, however, if we consider the transition through the bounce. The bounce connects a contracting and an expanding phase, each of which is described well by Wheeler–DeWitt evolution. In these phases, fluctuations relative to expectation values remain nearly constant.

During the transition through the bounce, however, the magnitude of fluctuations can change dramatically by factors, which do not need to be near 1 because fluctuations before and after the bounce are determined by independent free parameters of dynamical coherent states, as illustrated in Figure 10. The ratio of these parameters is related to the squeezing of the state of the universe [69]. For unsqueezed states, fluctuations before and after the bounce are symmetric, but this is an additional assumption for which no observational basis exists. While the uncertainty relation (74) restricts squeezing, and thus the asymmetry, for given fluctuations through a bound on the covariance, a controlled application would require tight control on fluctuations of isotropic variables of the universe.

If one were to ask whether the state before the Big Bang was as classical as the state after the Big Bang, this question could not be answered based solely on observational information available after the Big Bang; fluctuations before the bounce simply have such a weak influence that they could not be discerned from observations afterwards [72].[3] Moreover, the ratio of fluctuations before and after the bounce depends very sensitively on state parameters such that a state with symmetric fluctuations requires extreme fine tuning [74].

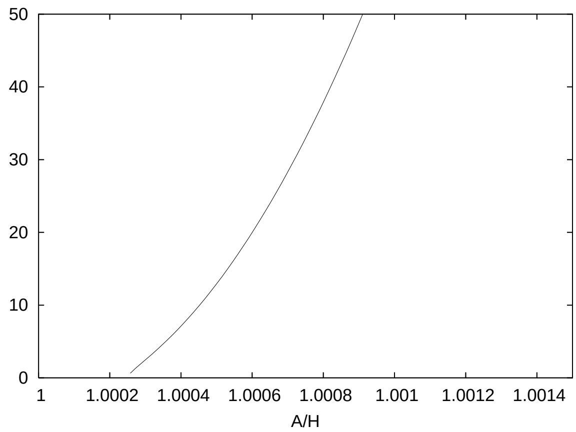

Figure 11: Ratio of fluctuations before (Δ_-) and after (Δ_+) the bounce in the form $|1-\Delta_-/\Delta_+|$ as a function of a state parameter A in relation to the Hamiltonian $H=\langle\hat{H}\rangle$ for $H=1000$ in Planck units. For larger H, the curve becomes even steeper, showing how precisely one has to tune the state parameter A in order to have a near symmetric state with $|1-\Delta_-/\Delta_+|=0$. See [74] for further details.

6.5.3 Physical inner product

As mentioned in Section 6.3, after solving effective equations one has to impose reality conditions to ensure that expectation values and fluctuations of observables are real. This is the same condition one requires to determine the physical inner product, which at the representation level can be very complicated. For solutions to effective equations, on the other hand, reality conditions are as straightforward to implement as in the classical case. In this way, physical inner product issues are under much better control in the effective treatment. This has been demonstrated not only for the exactly effective solvable system of a free scalar in a flat isotropic universe, but also in the

[3] In [138] the absolute rather than relative change of quadratic fluctuations before and after the bounce in a semiclassical state was found to be bounded from above by another fluctuation. While this does provide limits to the growth of fluctuations, the form of the inequality shows that strong relative changes even by factors much larger than discussed here are easily allowed by this analysis. Relative changes, which are less sensitive to the precise scale of fluctuations, were, however, not considered in [138].

presence of a perturbative potential [87], where quantum backreaction occurs. This issue is also important for the effective treatment of constrained systems.

6.5.4 Anomaly issue

In addition to the physical inner product, potential anomalies are one major issue in quantum gravity. Here also, though direct calculations for operators are hard to perform in general, effective constraints provide a much more practical route. One can first derive effective equations for a given set of constraint operators, not worrying about anomalies. Inconsistencies can only arise when one tries to solve the resulting effective constraints, so before doing so one must analyze the anomaly issue at the effective level. This is feasible because the effective constraints are of the classical type, although amended by quantum corrections. Calculations thus require only the use of Poisson relations rather than commutators of operators. Moreover, after effective constraints have been computed one can often incorporate systematic approximation schemes such as perturbation theory, and then make sure that anomalies are absent order by order. This is a further simplification, which has been used in several cases of quantum cosmological perturbation theory. As one of the results, the possibility of anomaly freedom in perturbative loop quantizations in the presence of non-trivial quantum corrections was demonstrated [92, 90, 91], and is studied for non-perturbative spherical symmetry in [102]. There are then standard techniques to compute evolution equations for gauge invariant observables from the anomaly-free effective constraints, which can immediately be employed in cosmological phenomenology.

These conclusions are also conceptually important for the general framework: the loop quantization does not necessarily remove covariance, as it is sometimes said. Non-trivial quantum corrections of the characteristic forms of loop quantum gravity are allowed while respecting covariance in effective equations. This issue is related to the question of local Lorentz invariance, although it has not been fully evaluated yet. Naive corrections in Hamiltonians or equations of motion could imply superluminal propagation, e.g., of gravitational waves. This would certainly violate causality, but superluminal motion disappears when anomaly freedom is properly implemented [91]. And yet, non-trivial quantum corrections due to the loop quantization remain.

7 Models within the Full Theory

If he uses a model at all, he is always aware that it pictures only certain aspects of the situation and leaves out other aspects. The total system of physics is no longer required to be such that all parts of its structure can be clearly visualized....

A physicist must always guard against taking a visual model as more than a pedagogical device or makeshift help. At the same time, he must also be alert to the possibility that a visual model can, and sometimes does, turn out to be literally accurate. Nature sometimes springs such surprises.

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In Section 5, the link between models and the full theory was given through a close relationship in the basic variables and the same kind of representation used, as well as a general construction scheme for the Hamiltonian constraint operator. The desired simplifications were realized thanks to the symmetry conditions, but not too strongly since basic features of the full theory are still recognizable in models. For instance, even though they would be possible in many ways and are often made use of, we did not employ special gauges or coordinate or field dependent transformations obscuring the relation. The models are thus as close to the full theory as possible while making full use of simplifications in order to have explicit applications.

Still, there are always some differences not all of which are easy to disentangle. For instance, we have discussed possible degeneracies between spin labels and edge lengths of holonomies, which can arise in the presence of a partial background and lead to new ambiguity parameters not present in the full theory. The question arises of what the precise relationship between models and the full theory is, or even how and to what extent a model for a given symmetry type can be derived from the full theory.

This is possible for the basic representation: the symmetry and the partial background it provides can be used to define natural sub-algebras of the full holonomy/flux algebra by using holonomies and fluxes along symmetry generators and averaging in a suitable manner. Since the full representation is unique and cyclic, it induces uniquely a representation of models that is taken directly from the full theory. This will now be described independently for states and basic operators in order to provide the idea and to demonstrate the role of the extra structure involved. See also [65] and [88] for illustrations in the context of spherical symmetry and anisotropy, respectively.

7.1 Symmetric states

One can imagine states that are invariant under a given action of a symmetry group on space by starting with a general state and naively summing over all its possible translates by elements of the symmetry group. For instance on spin network states, the symmetry group acts by moving the graph underlying the spin network, keeping the labels fixed. Since states with different graphs are orthogonal to each other, the sum over uncountably many different translates cannot be normalizable. In simple cases, such as for graphs with a single edge along a symmetry generator, one can easily make sense of the sum as a distribution. But this is not clear for arbitrary states, in particular for states whose graphs have vertices, which on the other hand would be needed for sufficient generality. A further problem is that any such action of a symmetry group is a subgroup of the diffeomorphism group. At least on compact space manifolds where there are no asymptotic conditions for diffeomorphisms in the gauge group, it then seems that any group-averaged diffeomorphism-invariant state would already be symmetric with respect to arbitrary symmetries, which is obviously not sensible.

In fact, symmetries and (gauge) diffeomorphisms are conceptually very different, even though mathematically they are both expressed by group actions on a space manifold. Gauge diffeomorphisms are generated by first class constraints of the theory, which in canonical quantum gravity are imposed in the Dirac manner [153] or following refined algebraic quantization [31], conveniently done by group averaging [223]. Symmetries, however, are additional conditions imposed on a given theory to extract a particular sector of special interest. They can also be formulated as constraints added to the theory, but these constraints must be second class for a well-defined framework: one obtains a consistent reduced theory, e.g., with a non-degenerate symplectic structure, only if configuration and momentum variables are required to be symmetric in the same (or dual) way.

In the case of gravity in Ashtekar variables, the symmetry type determines, along the lines of Appendix A, the form of invariant connections and densitized triads defining the phase space of the reduced model. At the quantum level, however, one cannot keep connections and triads on the same footing since a polarization is required. One usually uses the connection representation in loop quantum gravity such that states are functionals on the space of connections. In a minisuperspace quantization of the classically reduced model, states would then be functionals only of invariant connections for the given symmetry type. This suggests that one should define symmetric states in the full theory to be those states, whose support contains invariant connections as a dense subset [96, 46] (one requires only a dense subset because possible generalized connections must be allowed for). As such, they must necessarily be distributional, as already expected from the naive attempt at a construction. Symmetric states thus form a subset of the distributional space Cyl^*. In this manner, only the reduced degrees of freedom are relevant, i.e., the reduction is complete, and all of them are indeed realized, i.e., the reduction is not too strong. Moreover, an "averaging" map from a non-symmetric state to a symmetric one can easily be defined by restricting the non-symmetric state to the space of invariant connections and requiring it to vanish everywhere else.

This procedure defines states as functionals, but since there is no inner product on the full Cyl^* this does not automatically result in a Hilbert space. Appropriately defined subspaces of Cyl^*, nevertheless, often carry natural inner products, which is also the case here. In fact, since the reduced space of invariant connections can be treated by the same mathematical techniques as the full space, it carries an analog of the full Ashtekar–Lewandowski measure and this is indeed induced from the unique representation of the full theory. The only difference is that in general an invariant connection is not only determined by a reduced connection but also by scalar fields (see Appendix A). As in the full theory, this space $\mathcal{A}_{\mathrm{inv}}$ of reduced connections and scalars is compactified to the space $\bar{\mathcal{A}}_{\mathrm{inv}}$ of generalized invariant connections on which the reduced Hilbert space is defined. One thus arrives at the same Hilbert space for the subset of symmetric states in Cyl^* as used before for reduced models, e.g., using the Bohr compactification in isotropic models. The new ingredient now is that these states have meaning in the full theory as distributions, whose evaluation on normalizable states depends on the symmetry type and partial background structure used.

Whether or not the symmetric Hilbert space obtained in this manner is identical to the reduced loop quantization of Section 5 is not a matter of definition, but would be a result of the procedure. The support of a distribution is by definition a closed subset of the configuration space. If the set of generalized invariant connections of $\bar{\mathcal{A}}_{\mathrm{inv}}$ is not a closed subset of $\bar{\mathcal{A}}$, the support of symmetric distributional states would be larger than the space of invariant connections. In such a case, the reduction at the quantum level would give rise to more degrees of freedom than loop quantization of the classically reduced model. Whether or not this is the case and what such degrees of freedom could be is still open; the situation is rather subtle. While the classical space of invariant connections is embedded in the space of all connections, this is not the case for generalized connections [117]. It is thus not obvious, whether the space of invariant connections is closed or what its closure is.

Alternative reduction procedures that are not based on states, which require the connection to be symmetric, but on coherent states, are being studied in [163, 164]. This has been shown to work well for free quantum-field theories, where also the Hamiltonian operator of the reduced model can be derived from the full one. However, since the existence of dynamical coherent states for the free theory is exploited in the construction it remains unclear how general Hamiltonian operators can be reduced.

7.2 Basic operators

In the classical reduction, symmetry conditions are imposed on both connections and triads, but in our description so far, at the level of states, only connections have been taken into account. Configuration and momentum variables play different roles in any quantum theory since a polarization is necessary. As we based the construction on the connection representation, symmetric triads have to be implemented at the operator level. (There cannot be additional reduction steps at the state level since, as we already observed, states just implement the right number of reduced degrees of freedom.)

Classically, the reduction of phase-space functions is simply done by pull back to the reduced phase space. The flow generated by the reduced functions then necessarily stays in the reduced phase space and defines canonical transformations for the model. An analogous statement in the corresponding quantum theory would mean that the reduced state space would be fixed by full operators such that their action (or dual action on distributions) could directly be used in the model without further work. This, however, is not the case with the reduction performed so far. We have considered only connections in the reduction of states; and also classically a reduction to a subspace $\mathcal{A}_{\rm inv}\times\mathcal{E}$, where connections are invariant but not triads, would be incomplete. First, this would not define a phase space of its own with a non-degenerate symplectic structure. More important in this context is the fact that this subspace would not be preserved by the flow of reduced functions.

As an example (see also [60] for a different discussion in the spherically-symmetric model) we consider a diagonal homogeneous model, such as Bianchi I for simplicity, with connections of the form $A_a^i{\rm d}x^a=\tilde{c}_{(I)}\Lambda_I^i\omega^I$ and look at the flow generated by the full volume $V=\int{\rm d}^3x\sqrt{|\det E|}$. It is straightforward to evaluate the Poisson bracket

$$\{A_a^i(x),V\}=2\pi\gamma G\epsilon_{abc}\epsilon^{ijk}E_j^bE_k^c/\sqrt{|\det E|}$$

already used in Equation (13). A point on $\mathcal{A}_{\rm inv}\times\mathcal{E}$ characterized by $\tilde{c}_{(I)}\Lambda_I^i$ and an arbitrary triad thus changes infinitesimally by

$$\delta(\tilde{c}_{(I)}\Lambda_I^i)=2\pi\gamma G\epsilon_{Ibc}\epsilon^{ijk}E_j^bE_k^c/\sqrt{|\det E|}\,,$$

which does not preserve the invariant form. First, on the right-hand side we have arbitrary fields E such that $\delta(\tilde{c}_{(I)}\Lambda_I^i)$ is not homogeneous. Second, even if we would restrict ourselves to homogeneous E, $\delta(\tilde{c}_{(I)}\Lambda_I^i)$ would not be of the original diagonal form. This is the case only if $\delta(\tilde{c}_{(I)}\Lambda_I^i)=\Lambda_I^i\delta(\tilde{c}_{(I)})$, since only the $\tilde{c}_I$ are canonical variables. The latter condition is satisfied only if

$$\epsilon^{ijk}\Lambda_I^j\delta(\tilde{c}_{(I)}\Lambda_I^i)=4\pi\gamma G\epsilon_{Ibc}\Lambda_{(I)}^jE_i^bE_j^c/\sqrt{|\det E|}$$

vanishes, which is not the case in general. This condition is true only if $E_i^a\propto\Lambda_i^a$, i.e., if we restrict the triads to be of diagonal homogeneous form, just as the connections.

A reduction of only one part of the canonical variables is thus incomplete and leads to a situation in which most phase-space functions generate a flow that does not stay in the reduced space. Analogously, the dual action of full operators on symmetric distributional states does not in general map this space to itself. Thus, an arbitrary full operator maps a symmetric state to a non-symmetric one and cannot be used to define the reduced operator. In general, one needs a second reduction step that implements invariant triads at the level of operators by an appropriate projection of its action back to the symmetric space. This can be quite complicated, and fortunately there are special full operators adapted to the symmetry for which this step is not necessary.

From the above example it is clear that those operators must be linear in the momenta E^a_i, for otherwise, one would have a triad remaining after evaluating the Poisson bracket, which on $\mathcal{A}_{\rm inv}\times\mathcal{E}$ would not be symmetric everywhere. Fluxes are linear in the momenta, so we can try $p^K(z_0):=\int_{S_{z_0}}{\rm d}^2y\Lambda^k_{(K)}E^a_k\omega^K_a$ where S_{z_0} is a surface in the IJ-plane at position $z=z_0$ in the K-direction. By choosing a surface along symmetry generators X_I and X_J this expression is adapted to the symmetry, even though it is not fully symmetric yet since the position z_0 has to be chosen. Again, we compute the Poisson bracket

$$\{A^i_a(x),p^K(z_0)\}=8\pi\gamma G\Lambda^i_{(K)}\int_{S_{z_0}}\delta(x,y)\omega^K_a(y)\,{\rm d}^2y$$

resulting in

$$\delta(\tilde{c}_{(I)}\Lambda^i_I)=8\pi\gamma G\Lambda^i_I\delta(z,z_0)\,.$$

Here, also, the right-hand side is not homogeneous, but we have $\epsilon^{ijk}\Lambda^j_I\delta(\tilde{c}_{(I)}\Lambda^k_I)=0$ such that the diagonal form is preserved. The violation of homogeneity is expected since the flux is not homogeneous. This can easily be remedied by "averaging" the flux in the K-direction to

$$p^K:=\lim_{N\to\infty}N^{-1}\sum_{\alpha=1}^{N}p^K(\alpha N^{-1}L_0)\,,$$

where L_0 is the coordinate length of the K-direction if it is compact. For any finite N the expression is well defined and can directly be quantized, and the limit can be performed in a well-defined manner at the quantum level of the full theory.

Most importantly, the resulting operator preserves the form of symmetric states for the diagonal homogeneous model in its dual action, corresponding to the flux operator of the reduced model as used before. In averaging the full operator the partial background provided by the group action has been used, which is responsible for the degeneracy between edge length and spin in one reduced flux label. Similarly, one can obtain holonomy operators along the I-direction, which preserve the form of symmetric states after averaging them along the J and K directions (in such a way that the edge length is variable in the averaging limit). Thus, the dual action of full operators is sufficient to derive all basic operators of the model from the full theory [66]. (See [88] for a simpler illustration of the reduction from anisotropic to isotropic models.) The representation of states and basic operators, which was seen to be responsible for most effects in loop quantum cosmology, is thus directly linked to the full theory. An elaboration of this algebraic version of the symmetry reduction can be found in [207, 208], which also shows promise in extending the reduction to non-basic operators such as the Hamiltonian constraint. This, then, defines the cosmological sector of loop quantum gravity.

7.3 Quantization before reduction

When quantizing a model after a classical reduction, there is much freedom even in choosing the basic representation. For instance, in homogeneous models one can use the Wheeler–DeWitt formulation based on the Schrödinger representation of quantum mechanics. In other models one could choose different smearings, e.g., treating triad components by holonomies and connection components by fluxes, since transformation properties can change from the reduced point of view (see, e.g., [60]). There is, thus, no analog to the uniqueness theorem of the full theory, and models constructed in this manner would have much inherent freedom even at a basic level. With the link to the full theory, however, properties of the unique representation there are transferred directly to models, resulting in analogous properties such as discrete fluxes and an action only of exponentiated connection components. This is sufficient for a construction by analogy of composite operators, such as the Hamiltonian constraint according to the general scheme.

If the basic representation is taken from the full quantization, one makes sure that many consistency conditions of quantum gravity are already observed. This can never be guaranteed when classically reduced models are quantized since then many consistency conditions trivialize as a consequence of simplifications in the model. In particular, background independence requires special properties, as emphasized before. A symmetric model, however, always incorporates a partial background and, within a model alone, one cannot determine which structures are required for background independence. In loop quantum cosmology, on the other hand, this is realized thanks to the link to the full theory. Even though a model in loop quantum cosmology can also be seen as obtained by a particular minisuperspace quantization, it is distinguished by the fact that its representation is derived by quantizing before performing the reduction.

In general, symmetry conditions take the form of second-class constraints since they are imposed for both connections and triads. It is often said that second-class constraints always have to be solved classically before the quantization because of quantum uncertainty relations. This seems to make impossible the above statement that symmetry conditions can be imposed after quantizing. It is certainly true that there is no state in a quantum system satisfying all second class constraints of a given reduction. In addition, using distributional states, as required for first-class constraints with zero in the continuous spectrum, does not help. The reduction described above does not simply proceed in this way by finding states, normalizable or distributional, in the full quantization. Instead, the reduction is done at the operator algebra level, or, alternatively, the selection of symmetric states is accompanied by a reduction of operators which, at least for basic ones, can be performed explicitly. In general terms, one does not look for a sub-representation of the full quantum representation, but for a representation of a suitable sub-algebra of operators related to the symmetry. This gives a well-defined map from the full basic representation to a new basic representation of the model. In this map, non-symmetric degrees of freedom are removed irrespective of the uncertainty relations from the full point of view.

Since the basic representations of the full theory and the model are related, it is clear that similar ambiguities arise in the construction of composite operators. Some of them are inherited directly, such as the representation label j one can choose when connection components are represented through holonomies [170]. Other ambiguities are reduced in models since many choices can result in the same form or are restricted by adaptations to the symmetry. This is, for instance, the case for positions of new vertices created by the Hamiltonian constraint. However, new ambiguities can also arise from degeneracies, such as that between spin labels and edge lengths resulting in the parameter δ in Section 5.4. Factor ordering can also appear more ambiguously in a model and lead to less unique operators than in the full theory. As a simple example we can consider a system with two degrees of freedom $(q_1, p_1; q_2, p_2)$ constrained to be equal to each other: $C_1 = q_1 - q_2$, $C_2 = p_1 - p_2$. In the unconstrained plane (q_1, q_2), angular momentum is given by $J = q_1 p_2 - q_2 p_1$ with an unambiguous quantization. Classically, J vanishes on the constraint surface $C_1 = 0 = C_2$, but in the quantum system ambiguities arise: q_1 and p_2 commute before but not after reduction. There is thus a factor-ordering ambiguity in the reduction, which is absent in the unconstrained system. Since angular momentum operators formally appear in the volume operator of loop quantum gravity, it is not surprising that models have additional factor-ordering ambiguities in their volume operators. Fortunately, they are harmless and result, e.g., in differences as an isotropic volume spectrum $|\mu|^{3/2}$ compared to $\sqrt{(|\mu|-1)|\mu|(|\mu|+1)}$, where the second form [45] is closer to SU(2) as compared to U(1) expressions.

7.4 Minisuperspace approximation

Most physical applications in quantum gravity are obtained in mini- or midisuperspace truncations by focusing only on degrees of freedom relevant for a given situation of interest. Other degrees of freedom and their interactions with the remaining ones are ignored so as to simplify the complicated full dynamics. Their role, in particular for the evolution, however, is not always clear, and so one should check what happens if they are gradually tuned in.

There are examples, in the spirit of [210], where minisuperspace results are markedly different from less symmetric ones. In those analyses, however, already the classical reduction is unstable, or classical backreaction is important, and thus solutions that start almost symmetric move away rapidly from the symmetric sub-manifold of the full phase space. The failure of a minisuperspace quantization in those cases can already be decided classically and is not a quantum gravity issue. Even a violation of uncertainty relations, which occurs in any reduction at the quantum level, is not automatically dangerous, but only if corresponding classical models are unstable.

As for the general approach to a classical singularity, the anisotropic behavior, and not so much inhomogeneities, is considered to be essential. Isotropy can indeed be misleading, but the anisotropic behavior is more characteristic. In fact, relevant features of full calculations on a single vertex [120] agree with the anisotropic [56, 82], but not the isotropic behavior [54]. Also, patching together homogeneous models to form an inhomogeneous space reproduces some full results even at a quantitative level [100]. The main differences and simplifications of models can be traced back to an effective Abelianization of the full SU(2)-gauge transformations, which is not introduced by hand in this case but by a consequence of symmetries. It is also one of the reasons why geometrical configurations in models are usually easier to interpret than in the full theory. Most importantly, it implies strong conceptual simplifications since it allows a triad representation in which the dynamics can be understood more intuitively than in a connection representation. Explicit results in models have thus been facilitated by this property of basic variables, and therefore a comparison with analogous situations in the full theory is most interesting in this context, and most important as a test of models.

If one is using a quantization of a classically-reduced system, it can only be considered a model for full quantum gravity. Relations between different models and the full theory are important in order to specify to what degree such models approximate the full situation, and where additional correction terms from the ignored degrees of freedom have to be taken into account. This is under systematic investigation in loop quantum cosmology.

7.5 Quantum geometry: from models to the full theory

By now, many models are available explicitly and can be compared with each other and the full theory. Original investigations were done in isotropic models, which in many respects are special, but important aspects of the loop quantization are now known to be realized in all models and sometimes the full theory, without contradictions so far. Thus there is a consistent picture of singularity-free dynamical behavior together with candidates for characteristic phenomenology.

There are certainly differences between models, which can be observed already for geometrical spectra such as area or volume. Akin to level splitting in atoms or molecules, spectra become more complicated when symmetry is relaxed [96, 107, 95]. In addition, the behavior of densities or curvatures on arbitrary geometrical configurations can be different in different models. In isotropic models, densities are bounded, which is a kinematical statement, but in this case important for a singularity-free evolution. It is important here since minisuperspace is just one-dimensional and so dynamical trajectories could not pass regions of unbounded curvature, should they exist. Anisotropic models are more characteristic for the approach to classical singularities, and here curvature expressions in general remain unbounded if all of minisuperspace is considered. Again, this is only kinematical, and here the dynamics tells us that evolution does not proceed along directions of unbounded curvature. This is similar in inhomogeneous models studied so far.

In the full theory the situation again becomes more complicated since here densities can be unbounded, even on degenerate configurations of vanishing-volume eigenvalue [120]. In this case, however, it is not known what the significance for evolution is, or even the geometrical meaning of the degenerate configurations.

As an analogy one can, as before, take the spectroscopy of atoms and level splitting. Essential properties, such as the stability of the hydrogen atom in quantum mechanics as opposed to the classical theory, are unchanged if complicated interactions are taken into account. It is important to observe, in this context, that stability can and does change if arbitrary interactions are considered, rather than realistic ones, which one has already fixed from other observations. Hydrogen then remains stable under those realistic interactions, but its properties would change drastically if any possible interaction term were considered. Similarly, it is not helpful to consider the behavior of densities on arbitrary geometries unless it is known which configurations are important for dynamics or at least their geometrical role is clear. Dynamics in the canonical picture is encoded in the Hamiltonian constraint, and including it (or suitable observables) in the analysis is analogous, in the picture of atomic spectra, to making use of realistic gravitational interaction terms. In the full theory, such an analysis is currently beyond reach, but it has been extensively studied in loop quantum cosmology. Since the non-singular behavior of models, whether or not curvature is bounded, is a consequence of basic effects and the representation derived from the full theory, it can be taken as reliable information on the behavior in quantum geometry.

8 Philosophical Ramifications

In the context of loop quantum cosmology or loop quantum gravity in general, some wider issues arise that have already been touched upon briefly. This has to be seen in the general context of what one should expect from quantum theories of gravity, for which there are several quite different approaches. These issues deal with questions of the uniqueness of theories or solutions and what information is accessible in one universe. Also the role of time plays a more general role, and the related question of unitarity or determinism.

8.1 Unique theories, unique solutions

> *It is often the case that, before quantitative concepts can be introduced into a field of science, they are preceded by comparative concepts that are much more effective tools for describing, predicting, and explaining than the cruder classificatory concepts.*
>
> Rudolf Carnap
>
> An Introduction to the Philosophy of Science

The rise of loop quantum gravity presents an unprecedented situation in physics, in which full gravity is tackled in a background-independent and non-perturbative manner. Not surprisingly, the result is often viewed skeptically, since it is very different from other well-studied quantum field theories. Usually, intuition in quantum field theory comes either from models, which are so special that they are completely integrable, or from perturbative expansions around free field theories. Since no relevant ambiguities arise in this context, ambiguities in other frameworks are usually viewed with suspicion. A similar treatment is not possible for gravity because a complete formulation as a perturbation series around a free theory is unavailable and would anyway not be suitable in important situations of high curvature. In fact, reformulations as free theories exist only in special, non-dynamical backgrounds such as Minkowski space or planar waves, which, if used, immediately introduce a background.

If this is to be avoided in a background-independent formulation, it is necessary to deal with the full non-linear theory. This leads to complicated expressions with factor ordering and other ambiguities, which are usually avoided in quantum field theory but not unfamiliar from quantum theory in general. Sometimes it is said that such a theory loses its predictive power or it is even suggested that one stop working on applications of the theory until all ambiguities are eliminated. This view, of course, demonstrates a misunderstanding of the scientific process, in which general effects play important roles, even if they can be quantified only at later stages. What is important is to show that the qualitative effects are robust enough that their implications do not crucially depend on one choice among many.

So far, applications of loop quantum gravity and cosmology are in comparative stages, in which reliable effects can be derived from basic properties and remaining ambiguities preclude sharp quantitative predictions in general (notable exceptions are fundamental properties, such as the computation of γ through black-hole entropy [11, 12, 158, 225]). These ambiguities have to be constrained by further theoretical investigations of the overall consistency, or by possible observations.

Ambiguities certainly mean that a theory cannot be formulated uniquely, and uniqueness often plays a role in discussions of quantum gravity. In the many approaches different kinds of uniqueness have been advertised, most importantly the uniqueness of the whole theory, or the uniqueness of a solution appropriate for the one universe we can observe. Both expectations seem reasonable, though immodest. But they are conceptually very different and even, maybe surprisingly, inconsistent with each other as physical properties. For let us assume that we have a theory from which we know that it has one and only one solution. Provided that there is sufficient computational access to that theory, it is falsifiable by comparing properties of the solution with observations in the universe. Now, our observational access to the universe will always be limited and so, even if the one solution of our theory does agree with observations, we can always find ways to change the theory without being in observational conflict. The theory thus cannot be unique. Changing it in the described situation may only violate other, external conditions, which are not observable.

The converse, that a unique theory cannot have a unique solution, follows by logically reversing the above argument. However, one has to be careful about different notions of uniqueness of a theory. It is clear from the above argument that uniqueness of a theory can be realized only under external, such as mathematical, conditions, which always are a matter of taste and depend on existing knowledge. Nevertheless, the statement seems to be supported by current realizations of quantum gravity. String theory is one example, in which the supposed uniqueness of the theory is far outweighed by the non-uniqueness of its solutions. It should also be noted that the uniqueness of a theory is not falsifiable, and therefore not a scientific claim, unless its solutions are sufficiently restricted within the theory. Otherwise, one can always find new solutions if one comes in conflict with observations. A theory itself, however, is falsifiable if it implies characteristic effects for its solutions, even though it may otherwise be ambiguous.

8.2 The role of time

> *Dies alles dauerte eine lange Zeit, oder eine kurze Zeit: denn, recht gesprochen, gibt es für dergleichen Dinge auf Erden* keine Zeit.
>
> (*All this took a long time, or a short time: for, strictly speaking, for such things* no time *on earth exists.*)
>
> Friedrich Nietzsche
> Thus Spoke Zarathustra

Often, time is intuitively viewed as coordinate time, i.e., one direction of spacetime. However, this does not have invariant physical meaning in general relativity, and conceptually an internal time is more appropriate. Evolution is then measured in a relational manner of some degrees of freedom with respect to others [40, 252, 154]. In quantum cosmology, as we have seen, this concept is even more general, since internal time keeps making sense at the quantum level, even around singularities, where classical spacetime dissolves.

The wave function thus extends to a new branch beyond the classical singularity, i.e., to a classically disconnected region. Intuitively this leads to a picture of a collapsing universe preceding the Big Bang, but one has to keep in mind that this is the picture obtained from internal time, where other time concepts are not available. In such a situation it is not clear, intuitive pictures notwithstanding, how this transition would be perceived by observers, were they able to withstand the extreme conditions. It can be said reliably that the wave function is defined on both sides, "before" and "after", and every computation of physical predictions, e.g., using observables, that we can do at "our" side, can also be done at the other side. In this sense, quantum gravity is free of singularities and provides a transition between the two branches. The more complex question is what this means for the evolution in a literal sense of our usual concept of time (see also [298]).

Effective equations displaying bounces in internal or coordinate-time evolution indicate that indeed classical singularities are replaced by a bouncing behavior. However, this does not occur completely generally and does not say anything about the orientation reversal, which is characteristic for the quantum transition. In fact, effective equations describe the motion of semiclassical wave packets, which become less reliable at very small volume. And even if the effective bounce happens far away from the classical singularity, will there in general be a part of the wave function splitting off and traversing to the other orientation, as can be seen in the example of Figure 12.

It is not clear in general that a wave function penetrating a classical singularity enters a new classical regime, even if the volume becomes large again. For instance, there can be oscillations

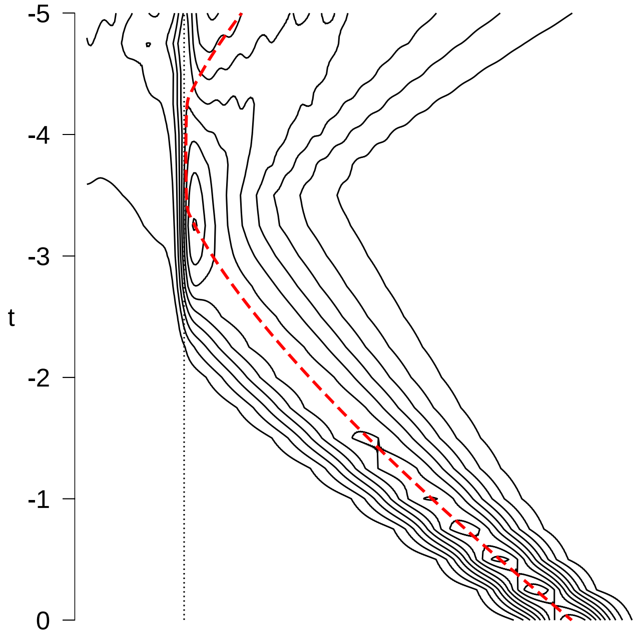

Figure 12: Still from a movie showing The coordinate time evolution [103] of a wave packet starting at the bottom and moving toward the classical singularity (vertical dotted line) for different values of an ambiguity parameter. Some part of the wave packet bounces back (and deforms) according to the effective classical solution (dashed), but other parts penetrate to negative μ. The farther away from $a = 0$ the effective bounce happens, depending on the ambiguity parameter, the smaller the part penetrating to negative μ is. The coordinate time evolution represents a physical state obtained after integrating over t [103]. (To watch the movie, please go to the online version of this review article at `http://www.livingreviews.org/lrr-2008-4`.)

on small scales, i.e., violations of pre-classicality, picked up by the wave function when it travels through the classical singularity. As discussed in Section 5.18, the question of what conditions to require on a wave function to require for a classical regime is still open, but even if one can confidently say that there is such a new classical region does the question arise if time continues during the transition through the pure quantum regime? At least in the special model of a free massless scalar in isotropic cosmology, the answer to both questions is affirmative, based on the availability of a physical inner product and quantum observables in this model [26]. More realistic models remain to be studied, which also must include parity-violating matter Hamiltonians, in which the difference equation would not be invariant under orientation reversal.

Also related to this context is the question of unitary evolution. Even if one uses a self-adjoint constraint operator, unitary evolution is not guaranteed. First, the constraint splits into a time-generator part containing derivatives or difference operators with respect to internal time and a source part containing, for instance, the matter Hamiltonian. It is then not guaranteed that the time generator will lead to unitary evolution. Secondly, it is not obvious in which inner product one should measure unitarity, since the constraint is formulated in the kinematical Hilbert space, but the physical inner product is relevant for its solutions. This shows that the usual expectation of unitary evolution, commonly motivated by the preservation of probability or the normalization of a wave function in an absolute time parameter, is not reliable in quantum cosmology. It must be replaced by suitable conditions on relational probabilities computed from physical wave functions.

8.3 Determinism

Hat die Zeit nicht Zeit? (*Does time not have time?*)

FRIEDRICH NIETZSCHE
Beyond Good and Evil

Loosely related to unitarity, but more general, is the concept of determinism. This is usually weakened in quantum mechanics anyway since in general one makes only probabilistic statements. Nevertheless, the wave function is determined at all times by its initial values, which is sometimes seen as the appropriate substitute for deterministic behavior. In loop quantum cosmology the situation again changes slightly since, as discussed in Section 5.19, the wave function may not be determined by the evolution equation everywhere, i.e., not at points of classical singularities, and instead may acquire new conditions on its initial values. This could be seen as a form of indeterministic behavior, even though the values of a wave function at classical singularities would not have any effect on the behavior of non-degenerate configurations.[4] (If they had such an effect, the evolution would be singular.) In this situation one deals with determinism in a background-independent context, which requires a new view.

In fact, rather than interpreting the freedom of choosing values at classical singularities as indeterministic behavior, it seems more appropriate to see this as an example for deterministic behavior in a background-independent theory. The internal time label μ first appears as a kinematical object through the eigenvalues of the triad operator (49). It then plays a role in the constraint equation (53) when formulated in the triad representation. Choosing internal time is just done for convenience, and it is the constraint equation that must be used to see if this choice makes sense in order to formulate evolution. This is indeed the case at non-zero μ, where we obtain a difference operator in the evolution parameter. At zero μ, however, the operator changes and does not allow us to determine the wave function there from previous values. Now, we can interpret this simply as a consequence of the constraint equation rejecting the internal time value $\mu = 0$. The background-independent evolution selects the values of internal time it needs in order to propagate a wave function uniquely. As it turns out, $\mu = 0$ is not always necessary for this

[4] The author thanks Christian Wüthrich for discussions.

and thus simply decouples. In hindsight, one could already have split off $|0\rangle$ from the kinematical Hilbert space, thereby removing the classical singularity by hand. Since we did not do this, it is the evolution equation that tells us that this is happening anyway. Recall, however, that this is only one possible scenario obtained from a non-symmetric constraint. For the evolution (55) following from the symmetric constraint, no decoupling happens and $\mu = 0$ is just like any other internal time value.

9 Research Lines

Currently, the development of loop quantum cosmology proceeds along different lines, at all levels discussed previously. We present here a list of the main ones, ordered by topics rather than importance or difficulty.

9.1 Conceptual issues

The list of conceptual issues is not much different from, but equally pressing as, quantum gravity in general. Here, mainly, the issue of time (its interpretation, different roles and explicit implementation into physics), the interpretation of the wave function in quantum theory, and technical as well as conceptual questions related to the physical inner product need to be addressed.

9.2 Mathematical development of models

The main open issue, requiring new insights at all levels, is that of inhomogeneities. While inhomogeneous models have been formulated and partly analyzed, the following tasks are still to be completed.

Exact models: In particular, the dynamics of inhomogeneous models is much more difficult to analyze than that of homogeneous ones. Understanding may be improved by an interesting cross-relation with black holes. This allows one to see if the different ingredients and effects of a loop quantization fit together in a complete picture, which so far seems to be the case [14, 233, 83, 13, 108, 65]. Moreover, the dynamics can possibly be simplified and understood better around slowly evolving horizons [113, 108]. Other horizon conditions are also being studied in related approaches [190, 155].

Consistency: Not directly related to physical applications, but equally important, is the issue of consistency of the constraints. The constraint algebra trivializes in homogeneous models, but is much more restrictive with inhomogeneities. Here, the feasibility of formulating a consistent theory of quantum gravity can be tested in a treatable situation. Effective treatments of constrained systems are beginning to shed valuable light on the anomaly issue and possible restrictions of quantization ambiguities by the condition of anomaly freedom. Related to consistency of the algebra, at least at a technical level, is the question of whether or not quantum gravity can predict initial conditions for a universe, or at least restrict its set of solutions.

Relationship between models and the full theory: By strengthening the relationship between models and the full theory, ideally providing a complete derivation of models, physical applications will be put on a much firmer footing. This is also necessary to understand better effects of reductions, such as degeneracies between different concepts or partial backgrounds. One aspect not realized in models so far is the large amount of non-Abelian effects in the full theory, which can be significant even in models [62].

Numerical quantum gravity: Most systems of difference equations arising in loop quantum gravity are too complicated to solve exactly or even to analyze. Special techniques, such as those in [103, 124, 101, 26, 130] have to be developed so as to apply them to more general systems. Isotropic models with a free massless scalar can be analyzed by efficient numerical techniques, but this is much more complicated for interacting matter or when several gravitational degrees of freedom are present. In the latter case, possible non-equidistancy may further complicate the analysis. In particular for inhomogeneities, both for solving equations and interpreting solutions, a new area of numerical quantum gravity has to be developed.

Perturbations: If the relationship between different models is known, as presently realized for isotropic models within homogeneous ones [88], one can formulate the less symmetric model perturbatively around the more symmetric one. This then provides a simpler formulation of the more complicated system, easing the analysis and uncovering new effects. In this context, alternative methods for introducing approximate symmetries, based on coherent states as, e.g., advocated in [119], also exist. Inhomogeneous perturbations have been formulated in [66] and are being developed for cosmological perturbation theory.

Effective equations: Finding effective equations that capture the quantum behavior of basic difference equations, at least in some regimes, will be most helpful for a general analysis. This is the place where probably the most unexpected progress has taken place over the last two years, leading to an exactly solvable isotropic model, which can be used as the "free" basis for a systematic perturbation analysis of more general systems. A derivation of effective equations is much more complicated for inhomogeneous systems, where it also has to be combined with an analysis of the consistency issue. On the other hand, such a derivation will provide important tests for the framework, in addition to giving rise to new applications.

9.3 Applications

Once available, equations for inhomogeneous systems have the prospect of applications such as the following.

Structure formation: There are diverse scenarios for the early universe with a potential for viable structure formation, which can only be checked with a reliable handle on inhomogeneities. This applies to inflaton models with loop effects, inflation models without inflaton, and the generation of structure before a bounce and subsequent propagation through it.

Robustness: All results obtained so far have to be regarded as preliminary and their validity in the presence of perturbative inhomogeneities has to be established. A detailed analysis of their robustness to quantization freedom such as ambiguities or choosing matter fields is still to be undertaken.

New effects: Some cosmological issues that have not been addressed in detail so far by loop quantum gravity, and which most likely require inhomogeneities, are: the initial state of the inflaton (Gaussianity) or the present acceleration of cosmic expansion. The latter has been suggested to be a result of small, local quantum corrections adding up to a sizeable effect on the whole universe [73]. From a technical point of view, closer contact to quantum gravity phenomenology in a particle physics context should be made (as initially in [100]), especially including anomaly freedom and analyzing the status of Lorentz symmetry.

Ansatzs: For the time being, these questions can be addressed preliminarily by choosing suitable forms of inhomogeneous equations motivated by operators in full loop quantum gravity.

9.4 Homogeneous models

There are still several open areas in homogeneous models, which can later be extended to inhomogeneous ones.

Conceptual issues: This has already been mentioned above. Isotropic models provide simpler settings to analyze, e.g., the physical inner product [184, 243, 26, 33], observables, different interpretations of quantum aspects or the emergence of a classical world.

Effective equations: Even in isotropic models, effective equations have only been derived completely in one special class of models [70]. A general scheme exists, shown to be analogous to standard effective-action techniques [105], but it remains to be applied in detail to quantum cosmology, as done for an interacting scalar in [87]. If successful, this will lead to a complete set of correction terms and their ranges of validity and importance. In addition, the question of whether a covariant effective action for quantum cosmology exists and what its form is can be addressed.

Properties of states: In some isotropic models, properties of dynamical coherent states are available [70, 69]. Thus, cosmological applications, which take into account the evolution of a full quantum state, rather than just classical variables subject to equations with quantum corrections, become possible. Quite surprisingly at first sight, state properties can change significantly in cosmological transitions, especially at the Big Bang, and play an important role for potential conclusions drawn from observations [72, 74]. This highlights the role of dynamical coherent states, which illustrate effects not visible for kinematical coherent states.

Matter systems: Matter systems provide a rich source of diverse scenarios, but a full analysis is yet to be done. This includes adding different kinds of fluids [244], fermions or anisotropy parameters (shear term).

9.5 Future work

All these developments will certainly aid and suggest insights into the full theory, and reciprocally be assisted by new ideas realized there. At the other end of the spectrum, guidance, as well as means for testing, can be expected from future observations.

A Invariant Connections

We first fix our notation by describing the additional structure provided by a given action of a symmetry group on a space manifold. This allows us to review the mathematical classification of principal fiber bundles carrying an action of a symmetry group and their invariant connections.

A.1 Partial backgrounds

To describe a theory of connections, we need to fix a principal fiber bundle $P(\Sigma, G, \pi)$ over the analytic base manifold Σ with compact structure group G. Let $S < \mathrm{Aut}(P)$ be a Lie symmetry subgroup of bundle automorphisms acting on the principal fiber bundle P. Using the bundle projection $\pi\colon P \to \Sigma$ we get a symmetry operation of S on Σ. For simplicity we will assume that all orbits of S are of the same type. If necessary we will have to decompose the base manifold into several orbit bundles $\Sigma_{(F)} \subset \Sigma$, where $F \cong S_x$ is the isotropy subgroup of S consisting of elements fixing a point x of the orbit bundle $\Sigma_{(F)}$ (isotropy subgroups for different points in $\Sigma_{(F)}$ are not identical but conjugate to each other). This amounts to a special treatment of possible symmetry axes or centers.

By restricting ourselves to one fixed orbit bundle we fix an isotropy subgroup $F \leq S$ up to conjugacy, and we require that the action of S on Σ is such that the orbits are given by $S(x) \cong S/F$ for all $x \in \Sigma$. This will be the case if S is compact but also in most other cases of physical interest. Moreover, we will have to assume later on that the coset space S/F is reductive [202, 203], i.e., that $\mathcal{L}S$ can be written as a direct sum $\mathcal{L}S = \mathcal{L}F \oplus \mathcal{L}F_\perp$ with $\mathrm{Ad}_F(\mathcal{L}F_\perp) \subset \mathcal{L}F_\perp$. If S is semi-simple, $\mathcal{L}F_\perp$ is the orthogonal complement of $\mathcal{L}F$ with respect to the Cartan–Killing metric on $\mathcal{L}S$. Further examples are provided by freely acting symmetry groups, in which case we have $F = \{1\}$, and semi-direct products of the form $S = N \rtimes F$, where $\mathcal{L}F_\perp = \mathcal{L}N$. The latter cases are relevant for homogeneous and isotropic cosmological models.

The base manifold can be decomposed as $\Sigma \cong \Sigma/S \times S/F$, where $\Sigma/S \cong B \subset \Sigma$ is the base manifold of the orbit bundle and can be realized as a sub-manifold B of Σ via a section in this bundle. As already noted in the main text, the action of a symmetry group on space introduces a partial background into the model. In particular, full diffeomorphism invariance is not preserved but reduced to diffeomorphisms only on the reduced manifold B. To see what kind of partial background we have in a model, it is helpful to contrast the mathematical definition of symmetry actions with the physical picture.

To specify an action of a group on a manifold, one has to give, for each group element, a map between space points satisfying certain conditions. Mathematically, each point is uniquely determined by labels, usually by coordinates in a chosen (local) coordinate system. The group action can then be written down in terms of maps of the coordinate charts, and there are compatibility conditions for maps expressed in different charts to ensure that the ensuing map on the manifold is coordinate independent. If we have active diffeomorphism invariance, however, individual points in space are not well defined. This leads to the common view that geometrical observables, such as the area of a surface, are, for physical purposes, not actually defined by integrating over a sub-manifold simply in parameter form, but over subsets of space defined by the values of matter fields [253, 251]. Since matter fields are subject to diffeomorphisms, just as the metric, area defined in such a manner is diffeomorphism invariant.

Similarly, orbits of the group action are not to be regarded as fixed sub-manifolds, but as being deformed by diffeomorphisms. Fixing a class of orbits filling the space manifold Σ corresponds to selecting a special coordinate system adapted to the symmetry. For instance, in a spherically-symmetric situation one usually chooses spherical coordinates (r, ϑ, φ), where $r > 0$ labels the orbits and ϑ and φ are angular coordinates and can be identified with some parameters of the symmetry group SO(3). In a Euclidean space the orbits can be embedded as spheres S^2 of constant curvature. Applying a diffeomorphism, however, will deform the spheres and they are in general only topological S^2. Physically, the orbits can be specified as level surfaces of matter fields, similar to specifying space points. This concept allows us to distinguish, in a diffeomorphism-invariant manner, between curves (such as edges of spin networks) that are tangential and curves that are transversal to the group orbits.

It is, however, not possible to label single points in a given orbit in such a physical manner, simply because we could not introduce the necessary matter fields without destroying the symmetry. Thus we have to use the action of the symmetry group, which provides us with additional structure, to label the points, e.g., by using the angular coordinates in the example above. A similar role is played by the embedding of the reduced manifold B into Σ by choosing a section of the orbit bundle, which provides a base point for each orbit (a north pole in the example of spherical symmetry). This amounts to a partial fixing of the diffeomorphism invariance by allowing only diffeomorphisms that respect the additional structure. The reduced diffeomorphism constraint will then, in general, require only invariance with respect to diffeomorphisms of the manifold B.

In a reduced model, a partial fixing of the diffeomorphism invariance does not cause problems because all fields are constant along the orbits anyway. However, if we study symmetric states as generalized states of the full theory, as in Section 7, we inevitably have to partially break the diffeomorphism invariance. The distributional evaluation of symmetric states and the dual action of basic operators thus depends on the partial background provided by the symmetry.

A.2 Classification of symmetric principal fiber bundles

Fields that are invariant under the action of a symmetry group S on space Σ are defined by a set of linear equations for invariant field components. Nevertheless, finding invariant fields in gauge theories is not always straightforward, since, in general, fields need to be invariant only up to gauge transformations, which depend on the symmetry transformation. An invariant connection, for instance, satisfies the equation

$$s^*A = g(s)^{-1}Ag(s) + g(s)^{-1}\mathrm{d}g(s) \tag{81}$$

with a local gauge transformation $g(s)$ for each $s \in S$. These gauge transformations are not arbitrary, since two symmetry transformations s_1 and s_2 applied one after another have to imply a gauge transformation with $g(s_2s_1)$ related to $g(s_1)$ and $g(s_2)$. However, this does not simply amount to a group homomorphism property and allowed maps $g\colon S \to G$ are not easily determined by group theory. Thus, even though, for a known map g, one simply has to solve a system of linear equations for A, finding appropriate maps g can be difficult. In most cases, the equations would not have any non-vanishing solution at all, which would certainly be insufficient for interesting reduced field theories.

In the earlier physics literature, invariant connections and other fields have indeed been determined by trial and error [135], but the same problem has been solved in the mathematical literature [202, 203, 116] in impressive generality. This uses the language of principal fiber bundles, which already provides powerful techniques. Moreover, the problem of solving one system of equations for A and $g(s)$ at the same time is split into two separate problems, which allows a more systematic approach. The first step is to realize that a connection, whose local 1-forms A on Σ are invariant up to gauge, is equivalent to a connection 1-form ω defined on the full fiber bundle P, which satisfies the simple invariance conditions $s^*\omega = \omega$ for all $s \in S$. This is indeed simpler to analyze, since we now have a set of linear equations for ω alone. However, even though hidden in the notation, the map $g\colon S \to G$ is still present. The invariance conditions for ω defined on P are well defined only if we know a lift from the original action of S on the base manifold Σ to the full bundle P. As with maps $g\colon S \to G$, there are several inequivalent choices for the lift, which have to be determined. The advantage of this procedure is that this can be done by studying symmetric principal fiber bundles, i.e., principal fiber bundles carrying the action of a symmetry group, independent of the behavior of connections. In a second step, one can then ask what form invariant connections on a given symmetric principal fiber bundle have.

We now discuss the first step of determining lifts for the symmetry action of S from Σ to P. Given a point $x \in \Sigma$, the action of the isotropy subgroup F yields a map $F\colon \pi^{-1}(x) \to \pi^{-1}(x)$ of the fiber over x, which commutes with the right action of G on the bundle. To each point $p \in \pi^{-1}(x)$ we can assign a group homomorphism $\lambda_p\colon F \to G$ defined by $f(p) =: p \cdot \lambda_p(f)$ for all $f \in F$. To verify this we first note that commutativity of the action of $S < \mathrm{Aut}(P)$ with right multiplication of G on P implies that we have the conjugate homomorphism $\lambda_{p'} = \mathrm{Ad}_{g^{-1}} \circ \lambda_p$ for a different point $p' = p \cdot g$ in the same fiber:

$$p' \cdot \lambda_{p'}(f) = f(p \cdot g) = f(p) \cdot g = (p \cdot \lambda_p(f)) \cdot g = p' \cdot \mathrm{Ad}_{g^{-1}} \lambda_p(f)\,.$$

This yields

$$(f_1 \circ f_2)(p) = f_1(p \cdot \lambda_p(f_2)) = (p \cdot \lambda_p(f_2)) \cdot \mathrm{Ad}_{\lambda_p(f_2)^{-1}} \lambda_p(f_1) = p \cdot (\lambda_p(f_1) \cdot \lambda_p(f_2))$$

demonstrating the homomorphism property. We thus obtain a map $\lambda\colon P \times F \to G, (p, f) \mapsto \lambda_p(f)$ obeying the relation $\lambda_{p \cdot g} = \mathrm{Ad}_{g^{-1}} \circ \lambda_p$.

Given a fixed homomorphism $\lambda\colon F \to G$, we can build the principal fiber sub-bundle

$$Q_\lambda(B, Z_\lambda, \pi_Q) := \{p \in P_{|B} : \lambda_p = \lambda\} \tag{82}$$

over the base manifold B, which as structure group has the centralizer

$$Z_\lambda := Z_G(\lambda(F)) = \{g \in G : gf = fg \quad \text{for all} \quad f \in \lambda(F)\}$$

of $\lambda(F)$ in G. $P_{|B}$ is the restricted fiber bundle over B. A conjugate homomorphism $\lambda' = \mathrm{Ad}_{g^{-1}} \circ \lambda$ simply leads to an isomorphic fiber bundle.

The structure elements $[\lambda]$ and Q classify symmetric principal fiber bundles according to the following theorem [116]:

Theorem 1 *An S-symmetric principal fiber bundle $P(\Sigma, G, \pi)$ with isotropy subgroup $F \leq S$ of the action of S on Σ is uniquely characterized by a conjugacy class $[\lambda]$ of homomorphisms $\lambda\colon F \to G$ together with a* reduced bundle *$Q(\Sigma/S, Z_G(\lambda(F)), \pi_Q)$.*

Given two groups, F and G, we can make use of the relation [115]

$$\mathrm{Hom}(F, G)/\mathrm{Ad} \cong \mathrm{Hom}(F, T(G))/W(G) \tag{83}$$

in order to determine all conjugacy classes of homomorphisms $\lambda\colon F \to G$. Here, $T(G)$ is a maximal torus and $W(G)$ the Weyl group of G. Different conjugacy classes correspond to different sectors of the theory, which can be interpreted as having different topological charge. In spherically-symmetric electromagnetism, for instance, this is just magnetic charge [43, 96].

A.3 Classification of invariant connections

Now let ω be an S-invariant connection on the symmetric bundle P classified by $([\lambda], Q)$, i.e., $s^*\omega = \omega$ for any $s \in S$. After restriction, ω induces a connection $\tilde{\omega}$ on the reduced bundle Q. Because of the S-invariance of ω, the reduced connection $\tilde{\omega}$ is a 1-form on Q with values in the Lie algebra of the reduced structure group. To see this, fix a point $p \in P$ and a vector v in T_pP, such that $\pi_* v \in \sigma_* T_{\pi(p)} B$, where σ is the embedding of B into Σ. Such a vector, which does not have components along symmetry orbits, is fixed by the action of the isotropy group: $\mathrm{d}f(v) = v$.

The pull back of ω by $f \in F$ applied to v is by definition $f^\star \omega_p(v) = \omega_{f(p)}(\mathrm{d}f(v)) = \omega_{f(p)}(v)$. Now using the fact that f acts as gauge transformation in the fibers and observing the definition of λ_p and the adjoint transformation of ω, we obtain $\omega_{f(p)}(v) = \mathrm{Ad}_{\lambda_p(f)^{-1}}\omega_p(v)$. By assumption, the connection ω is S-invariant implying $f^\star\omega_p(v) = \mathrm{Ad}_{\lambda_p(f)^{-1}}\omega_p(v) = \omega_p(v)$ for all $f \in F$. This shows that $\omega_p(v) \in \mathcal{L}Z_G(\lambda_p(F))$, and ω can be restricted to a connection on the bundle Q_λ with structure group Z_λ.

Furthermore, using ω we can construct the linear map $\Lambda_p \colon \mathcal{L}S \to \mathcal{L}G, X \mapsto \omega_p(\tilde{X})$ for any $p \in P$. Here, $\tilde{X}$ is the vector field on P given by $\tilde{X}(h) := \mathrm{d}(\exp(tX)^\star h)/\mathrm{d}t|_{t=0}$ for any $X \in \mathcal{L}S$ and $h \in C^1(P, \mathbb{R})$. For $X \in \mathcal{L}F$ the vector field $\tilde{X}$ is a vertical vector field, and we have $\Lambda_p(X) = \mathrm{d}\lambda_p(X)$, where $\mathrm{d}\lambda \colon \mathcal{L}F \to \mathcal{L}G$ is the derivative of the homomorphism defined above. This component of Λ is therefore already given by the classifying structure of the principal fiber bundle. Using a suitable gauge, λ can be held constant along B. The remaining components $\Lambda_p|_{\mathcal{L}F_\perp}$ yield information about the invariant connection ω. They are subject to the condition

$$\Lambda_p(\mathrm{Ad}_f(X)) = \mathrm{Ad}_{\lambda_p(f)}(\Lambda_p(X)) \quad \text{for} \quad f \in F, X \in \mathcal{L}S\,, \tag{84}$$

which follows from the transformation of ω under the adjoint representation and which provides a set of equations determining the form of the components Λ.

Keeping only the information characterizing ω we have, besides $\tilde{\omega}$, the scalar field $\tilde{\phi} \colon Q \to \mathcal{L}G \otimes \mathcal{L}F_\perp^\star$, which is determined by $\Lambda_p|_{\mathcal{L}F_\perp}$ and can be regarded as having $\dim \mathcal{L}F_\perp$ components of $\mathcal{L}G$-valued scalar fields. The reduced connection and the scalar field suffice to characterize an invariant connection [116]:

Theorem 2 (Generalized Wang Theorem) *Let $P(\Sigma, G)$ be an S-symmetric principal fiber bundle classified by $([\lambda], Q)$ according to Theorem 1, and let ω be an S-invariant connection on P. Then the connection ω is uniquely classified by a* reduced connection *$\tilde{\omega}$ on Q and a* scalar field *$\tilde{\phi} \colon Q \times \mathcal{L}F_\perp \to \mathcal{L}G$ obeying Equation (84).*

In general, $\tilde{\phi}$ transforms under some representation of the reduced structure group Z_λ; its values lie in the subspace of $\mathcal{L}G$ determined by Equation (84) and form a representation space for all group elements of G (which act on Λ), whose action preserves the subspace. These are, by definition, precisely elements of the reduced group.

The connection ω can be reconstructed from its classifying structure $(\tilde{\omega}, \tilde{\phi})$ as follows. According to the decomposition $\Sigma \cong B \times S/F$ we have

$$\omega = \tilde{\omega} + \omega_{S/F}\,, \tag{85}$$

where $\omega_{S/F}$ is given by $\Lambda \circ \iota^\star \theta_{\mathrm{MC}}$ in a gauge depending on the (local) embedding $\iota \colon S/F \hookrightarrow S$. Here θ_{MC} is the Maurer–Cartan form on S taking values in $\mathcal{L}S$. Through Λ, ω depends on λ and $\tilde{\phi}$.

B Examples

With these general results we can now quickly derive the form of invariant connections for the cases studied in the main text.

B.1 Homogeneous models

In Bianchi models the transitive symmetry group acts freely on Σ, which implies that Σ can locally be identified with the group manifold S. The three generators of $\mathcal{L}S$ will be denoted as T_I, $1 \leq I \leq 3$, with relations $[T_I, T_J] = C^K_{IJ} T_K$, where C^K_{IJ} are the structure constants of $\mathcal{L}S$ fulfilling $C^J_{IJ} = 0$ for class A models by definition. The Maurer–Cartan form on S is given by $\theta_{\mathrm{MC}} = \omega^I T_I$ with left-invariant 1-forms ω^I on S, which fulfill the Maurer–Cartan equations

$$\mathrm{d}\omega^I = -\tfrac{1}{2} C^I_{JK} \omega^J \wedge \omega^K \,. \tag{86}$$

Due to $F = \{1\}$, all homomorphisms $\lambda\colon F \to G$ are given by $1 \mapsto 1$, and we can use the embedding $\iota = \mathrm{id}\colon S/F \hookrightarrow S$. An invariant connection then takes the form $A = \tilde{\phi} \circ \theta_{\mathrm{MC}} = \tilde{\phi}^i_I \tau_i \omega^I = A^i_a \tau_i \mathrm{d}x^a$ with matrices τ_i generating $\mathcal{L}\mathrm{SU}(2)$. The scalar field is given by $\tilde{\phi}\colon \mathcal{L}S \to \mathcal{L}G, T_I \mapsto \tilde{\phi}(T_I) =: \tilde{\phi}^i_I \tau_i$ already in its final form, because condition (84) is empty for a trivial isotropy group.

Using left-invariant vector fields X_I obeying $\omega^I(X_J) = \delta^I_J$ and with Lie brackets $[X_I, X_J] = C^K_{IJ} X_K$ the momenta canonically conjugate to $A^i_a = \tilde{\phi}^i_I \omega^I_a$ can be written as $E^a_i = \sqrt{g_0}\, \tilde{p}^I_i X^a_I$ with $\tilde{p}^I_i$ being canonically conjugate to $\tilde{\phi}^i_I$. Here, $g_0 = \det(\omega^I_a)^2$ is the determinant of the left-invariant metric $(g_0)_{ab} := \sum_I \omega^I_a \omega^I_b$ on Σ, which is used to provide the density weight of E^a_i. The symplectic structure can be derived from

$$\frac{1}{8\pi\gamma G} \int_\Sigma \mathrm{d}^3x\, \dot{A}^i_a E^a_i = \frac{1}{8\pi\gamma G} \int_\Sigma \mathrm{d}^3x\, \sqrt{g_0}\, \dot{\tilde{\phi}}^i_I \tilde{p}^J_i \omega^I(X_J) = \frac{V_0}{8\pi\gamma G} \dot{\tilde{\phi}}^i_I \tilde{p}^I_i \,,$$

to obtain

$$\{\tilde{\phi}^i_I, \tilde{p}^J_j\} = 8\pi\gamma G V_0 \delta^i_j \delta^J_I \tag{87}$$

with the volume $V_0 := \int_\Sigma \mathrm{d}^3x \sqrt{g_0}$ of Σ measured with the invariant metric g_0.

It is convenient to absorb the coordinate volume V_0 into the fields by redefining $\phi^i_I := V_0^{1/3} \tilde{\phi}^i_I$ and $p^I_i := V_0^{2/3} \tilde{p}^I_i$. This makes the symplectic structure independent of V_0 in accordance with background independence. These redefined variables automatically appear in holonomies and fluxes through coordinate integrations.

B.2 Isotropic models

On Bianchi models, additional symmetries can be imposed, which corresponds to a further symmetry reduction and introduces non-trivial isotropy subgroups. These models with enhanced symmetry can be treated on an equal footing by writing the symmetry group as a semi-direct product $S = N \rtimes_\rho F$, with the isotropy subgroup F and the translational subgroup N, which is one of the Bianchi groups. Composition in this group is defined as $(n_1, f_1)(n_2, f_2) := (n_1 \rho(f_1)(n_2), f_1 f_2)$, which depends on the group homomorphism $\rho\colon F \to \mathrm{Aut}N$ into the automorphism group of N (which will be denoted by the same letter as the representation on $\mathrm{Aut}\mathcal{L}N$ used below). Inverse elements are given by $(n, f)^{-1} = (\rho(f^{-1})(n^{-1}), f^{-1})$. To determine the form of the invariant connections we have to compute the Maurer–Cartan form on S (using the usual notation):

$$\begin{aligned}
\theta^{(S)}_{\mathrm{MC}}(n, f) &= (n, f)^{-1} \mathrm{d}(n, f) = (\rho(f^{-1})(n^{-1}), f^{-1})(\mathrm{d}n, \mathrm{d}f) \\
&= (\rho(f^{-1})(n^{-1}) \rho(f^{-1})(\mathrm{d}n), f^{-1}\mathrm{d}f) = (\rho(f^{-1})(n^{-1}\mathrm{d}n), f^{-1}\mathrm{d}f) \\
&= \left(\rho(f^{-1})(\theta^{(N)}_{\mathrm{MC}}(n)), \theta^{(F)}_{\mathrm{MC}}(f)\right) \,.
\end{aligned} \tag{88}$$

Here the Maurer–Cartan forms $\theta^{(N)}_{\rm MC}$ on N and $\theta^{(F)}_{\rm MC}$ on F appear. We then choose an embedding $\iota\colon S/F=N\hookrightarrow S$, which can most easily be done as $\iota\colon n\mapsto(n,1)$. Thus, $\iota^*\theta^{(S)}_{\rm MC}=\theta^{(N)}_{\rm MC}$, and a reconstructed connection takes the form $\tilde{\phi}\circ\iota^*\theta^{(S)}_{\rm MC}=\tilde{\phi}^i_I\omega^I\tau_i$, which is the same as for anisotropic models before (where now ω^I are left-invariant 1-forms on the translation group N). However, here $\tilde{\phi}$ is constrained by Equation (84) and we get only a subset as isotropic connections.

To solve Equation (84) we have to treat LRS (locally rotationally symmetric) models with a single rotational symmetry and isotropic models separately. In the first case we choose $\mathcal{L}F=\langle\tau_3\rangle$, whereas in the second case we have $\mathcal{L}F=\langle\tau_1,\tau_2,\tau_3\rangle$ ($\langle\cdot\rangle$ denotes the linear span). Equation (84) can be written infinitesimally as

$$\tilde{\phi}({\rm ad}_{\tau_i}(T_I))={\rm ad}_{{\rm d}\lambda(\tau_i)}\tilde{\phi}(T_I)=[{\rm d}\lambda(\tau_i),\tilde{\phi}(T_I)]$$

($i=3$ for LRS, $1\leq i\leq 3$ for isotropy). The T_I are generators of $\mathcal{L}N=\mathcal{L}F_\perp$, on which the isotropy subgroup F acts by rotation, ${\rm ad}_{\tau_i}(T_I)=\epsilon_{iIK}T_K$. This is the derivative of the representation ρ defining the semi-direct product S: conjugation on the left-hand side of (84) is ${\rm Ad}_{(1,f)}(n,1)=(1,f)(n,1)(1,f^{-1})=(\rho(f)(n),1)$, which follows from the composition in S.

Next, we have to determine the possible conjugacy classes of homomorphisms $\lambda\colon F\to G$. For LRS models their representatives are given by

$$\lambda_k\colon {\rm U}(1)\to{\rm SU}(2),\quad \exp t\tau_3\mapsto\exp kt\tau_3$$

for $k\in{}_0=\{0,1,\ldots\}$ (as will be shown in detail below for spherically-symmetric connections). For the components $\tilde{\phi}^i_I$ of $\tilde{\phi}$ defined by $\tilde{\phi}(T_I)=\tilde{\phi}^i_I\tau_i$, Equation (84) takes the form $\epsilon_{3IK}\tilde{\phi}^j_K=k\epsilon_{3lj}\tilde{\phi}^l_I$. This has a non-trivial solution only for $k=1$, in which case $\tilde{\phi}$ can be written as

$$\tilde{\phi}_1=\tilde{a}\tau_1+\tilde{b}\tau_2\,,\qquad \tilde{\phi}_2=-\tilde{b}\tau_1+\tilde{a}\tau_2\,,\qquad \tilde{\phi}_3=\tilde{c}\tau_3$$

with arbitrary numbers $\tilde{a}$, $\tilde{b}$, $\tilde{c}$ (the factors of $2^{-\frac{1}{2}}$ are introduced for the sake of normalization). Their conjugate momenta take the form

$$\tilde{p}^1=\tfrac{1}{2}(\tilde{p}_a\tau_1+\tilde{p}_b\tau_2),\qquad \tilde{p}^2=\tfrac{1}{2}(-\tilde{p}_b\tau_1+\tilde{p}_a\tau_2),\qquad \tilde{p}^3=\tilde{p}_c\tau_3,$$

and the symplectic structure is given by

$$\{\tilde{a},\tilde{p}_a\}=\{\tilde{b},\tilde{p}_b\}=\{\tilde{c},\tilde{p}_c\}=8\pi\gamma GV_0$$

and vanishes in all other cases. There is remaining gauge freedom from the reduced structure group $Z_\lambda\cong{\rm U}(1)$, which rotates the pairs $(\tilde{a},\tilde{b})$ and $(\tilde{p}_a,\tilde{p}_b)$. Then only $\sqrt{\tilde{a}^2+\tilde{b}^2}$ and its momentum $(\tilde{a}\tilde{p}_a+\tilde{b}\tilde{p}_b)/\sqrt{\tilde{a}^2+\tilde{b}^2}$ are gauge invariant.

In the case of isotropic models we have only two homomorphisms $\lambda_0\colon{\rm SU}(2)\to{\rm SU}(2), f\mapsto 1$ and $\lambda_1={\rm id}$ up to conjugation (to simplify notation we use the same letters for the homomorphisms as in the LRS case, which is justified by the fact that the LRS homomorphisms are restrictions of those appearing here). Equation (84) takes the form $\epsilon_{iIK}\tilde{\phi}^j_K=0$ for λ_0 without non-trivial solutions, and $\epsilon_{iIK}\tilde{\phi}^j_K=\epsilon_{ilj}\tilde{\phi}^l_I$ for λ_1. Each of the last equations has the same form as for LRS models with $k=1$, and their solution is $\tilde{\phi}^i_I=\tilde{c}\delta^i_I$ with an arbitrary $\tilde{c}$. In this case the conjugate momenta can be written as $\tilde{p}^I_i=\tilde{p}\delta^I_i$ and we have the symplectic structure $\{\tilde{c},\tilde{p}\}=\frac{8\pi}{3}G\gamma V_0$.

Thus, in both cases there is a unique non-trivial sector, and no topological charge appears. The symplectic structure can again be made independent of V_0 by redefining $a:=V_0^{1/3}\tilde{a}$, $b:=V_0^{1/3}\tilde{b}$, $c:=V_0^{1/3}\tilde{c}$ and $p_a:=V_0^{2/3}\tilde{p}_a$, $p_b:=V_0^{2/3}\tilde{p}_b$, $p_c:=V_0^{2/3}\tilde{p}_c$, $p:=V_0^{2/3}\tilde{p}$. If one computes the isotropic reduction of a Bianchi IX metric following from the left-invariant 1-forms of SU(2), one obtains a closed Friedmann–Robertson–Walker metric with scale factor $a=2\tilde{a}=2\sqrt{|\tilde{p}|}$ (see [44] for the calculation). Thus, we obtain identification (19) used in isotropic loop cosmology. (Such a normalization can only be obtained in curved models.)

B.3 Spherical symmetry

In the generic case, i.e., outside a symmetry center, of spherical symmetry we have $S = \mathrm{SU}(2)$, $F = \mathrm{U}(1) = \exp\langle\tau_3\rangle$ ($\langle\cdot\rangle$ denotes the linear span), and the connection form can be gauged to be

$$A_{S/F} = (\Lambda(\tau_2)\sin\vartheta + \Lambda(\tau_3)\cos\vartheta)\,\mathrm{d}\varphi + \Lambda(\tau_1)\mathrm{d}\vartheta\,. \tag{89}$$

Here, (ϑ, φ) are (local) coordinates on $S/F \cong S^2$ and, as usual, we use the basis elements τ_i of $\mathcal{L}S$. $\Lambda(\tau_3)$ is given by $\mathrm{d}\lambda$, whereas $\Lambda(\tau_{1,2})$ are the scalar field components. Equation (89) contains, as special cases, the invariant connections found in [135]. These are gauge equivalent by gauge transformations depending on the angular coordinates (ϑ, φ), i.e., they correspond to homomorphisms λ, which are not constant on the orbits of the symmetry group.

In order to specify the general form (89) further, the first step is again to find all conjugacy classes of homomorphisms $\lambda\colon F = \mathrm{U}(1) \to \mathrm{SU}(2) = G$. To do so, we can make use of Equation (83), to which end we need the following information about SU(2) (see, e.g., [115]). The standard maximal torus of SU(2) is given by

$$T(\mathrm{SU}(2)) = \{\mathrm{diag}(z, z^{-1}) : z \in \mathrm{U}(1)\} \cong \mathrm{U}(1)$$

and the Weyl group of SU(2) is the permutation group of two elements, $W(\mathrm{SU}(2)) \cong S_2$, its generator acting on $T(\mathrm{SU}(2))$ by $\mathrm{diag}(z, z^{-1}) \mapsto \mathrm{diag}(z^{-1}, z)$.

All homomorphisms in $\mathrm{Hom}(\mathrm{U}(1), T(\mathrm{SU}(2)))$ are given by

$$\lambda_k\colon z \mapsto \mathrm{diag}(z^k, z^{-k})$$

for any $k \in \mathbb{Z}$, and we have to divide out the action of the Weyl group leaving only the maps λ_k, $k \in \mathbb{N}_0$, as representatives of all conjugacy classes of homomorphisms. We see that spherically-symmetric gravity has a topological charge taking values in $\mathbb{N}_0$ (but only if degenerate configurations are allowed, as we will see below).

We will represent F as the subgroup $\exp\langle\tau_3\rangle < \mathrm{SU}(2)$ of the symmetry group S, and use the homomorphisms $\lambda_k\colon \exp t\tau_3 \mapsto \exp kt\tau_3$ out of each conjugacy class. This leads to a reduced-structure group $Z_G(\lambda_k(F)) = \exp\langle\tau_3\rangle \cong \mathrm{U}(1)$ for $k \neq 0$ and $Z_G(\lambda_0(F)) = \mathrm{SU}(2)$ ($k = 0$; this is the sector of manifestly invariant connections of [136]). The map $\Lambda|_{\mathcal{L}F}$ is given by $\mathrm{d}\lambda_k\colon \langle\tau_3\rangle \to \mathcal{L}G, \tau_3 \mapsto k\tau_3$, and the remaining components of Λ, which give us the scalar field, are determined by $\Lambda(\tau_{1,2}) \in \mathcal{L}G$ subject to Equation (84), which here can be written as

$$\Lambda \circ \mathrm{ad}_{\tau_3} = \mathrm{ad}_{\mathrm{d}\lambda(\tau_3)} \circ \Lambda\,.$$

Using $\mathrm{ad}_{\tau_3}\tau_1 = \tau_2$ and $\mathrm{ad}_{\tau_3}\tau_2 = -\tau_1$ we obtain

$$\Lambda(a_0\tau_2 - b_0\tau_1) = k(a_0[\tau_3, \Lambda(\tau_1)] + b_0[\tau_3, \Lambda(\tau_2)])\,,$$

where $a_0\tau_1 + b_0\tau_2$, $a_0, b_0 \in \mathbb{R}$ is an arbitrary element of $\mathcal{L}F_\perp$. Since a_0 and b_0 are arbitrary, this is equivalent to the two equations

$$k[\tau_3, \Lambda(\tau_1)] = \Lambda(\tau_2)\,, \qquad k[\tau_3, \Lambda(\tau_2)] = -\Lambda(\tau_1)\,.$$

A general ansatz

$$\Lambda(\tau_1) = a_1\tau_1 + b_1\tau_2 + c_1\tau_3\,, \quad \Lambda(\tau_2) = a_2\tau_1 + b_2\tau_2 + c_2\tau_3$$

with arbitrary parameters $a_i, b_i, c_i \in \mathbb{R}$ yields

$$k(a_1\tau_2 - b_1\tau_1) = a_2\tau_1 + b_2\tau_2 + c_2\tau_3\,,$$
$$k(-a_2\tau_2 + b_2\tau_1) = a_1\tau_1 + b_1\tau_2 + c_1\tau_3\,,$$

which have non-trivial solutions only if $k = 1$, namely

$$b_2 = a_1\,, \quad a_2 = -b_1 \quad \text{and} \quad c_1 = c_2 = 0\,.$$

The configuration variables of the system are the above fields $a, b, c : B \to \mathbb{R}$ of the U(1)-connection form $A = c(x)\,\tau_3\,\mathrm{d}x$ on the one hand and the two scalar-field components

$$\begin{aligned}\Lambda|_{\langle\tau_1\rangle} &: B \to \mathcal{L}\mathrm{SU}(2),\\ x &\mapsto a(x)\tau_1 + b(x)\tau_2 = \frac{1}{2}\begin{pmatrix} 0 & -b(x) - ia(x) \\ b(x) - ia(x) & 0 \end{pmatrix} =: \begin{pmatrix} 0 & -\overline{w}(x) \\ w(x) & 0 \end{pmatrix}\end{aligned}$$

on the other hand. Under a local U(1)-gauge transformation $z(x) = \exp(t(x)\tau_3)$ they transform as $c \mapsto c + \mathrm{d}t/\mathrm{d}x$ and $w(x) \mapsto \exp(-it)w$, which can be read off from

$$\begin{aligned} A &\mapsto z^{-1}Az + z^{-1}\mathrm{d}z = A + \tau_3\mathrm{d}t\,,\\ \Lambda(\tau_1) &\mapsto z^{-1}\Lambda(\tau_1)z = \begin{pmatrix} 0 & -\exp(it)\overline{w} \\ \exp(-it)w & 0 \end{pmatrix}\,. \end{aligned}$$

In order to obtain a standard symplectic structure (see Equation (92) below), we reconstruct the general invariant connection form

$$\begin{aligned} A(x,\vartheta,\varphi) = {} & A_1(x)\tau_3\mathrm{d}x + (A_2(x)\tau_1 + A_3(x)\tau_2)\mathrm{d}\vartheta \\ & + (A_2(x)\tau_2 - A_3(x)\tau_1)\sin\vartheta\,\mathrm{d}\varphi + \cos\vartheta\,\mathrm{d}\varphi\,\tau_3\,. \end{aligned} \tag{90}$$

An invariant densitized-triad field is analogously given by

$$(E^x, E^\vartheta, E^\varphi) = (E^1\sin\vartheta\,\tau_3, \tfrac{1}{2}\sin\vartheta(E^2\tau_1 + E^3\tau_2), \tfrac{1}{2}(E^2\tau_2 - E^3\tau_1)) \tag{91}$$

with coefficients E^I canonically conjugate to A_I (E^2 and E^3 are non-vanishing only for $k = 1$). The symplectic structure

$$\{A_I(x), E^J(y)\} = 2\gamma G\delta_I^J\delta(x,y) \tag{92}$$

can be derived by inserting the invariant expressions into $(8\pi\gamma G)^{-1}\int_\Sigma \mathrm{d}^3x\dot{A}_a^iE_i^a$.

Information about the topological charge k can be found by expressing the volume in terms of the reduced triad coefficients E^I. Using

$$\epsilon_{abc}\epsilon^{ijk}E_i^aE_j^bE_k^c = -2\epsilon_{abc}\mathrm{tr}(E^a[E^b,E^c]) = \tfrac{3}{2}\sin^2\vartheta E^1\left((E^2)^2 + (E^3)^2\right) \tag{93}$$

we have

$$V = \int_\Sigma \mathrm{d}^3x\sqrt{\tfrac{1}{6}\left|\epsilon_{abc}\epsilon^{ijk}E_a^iE_b^jE_c^k\right|} = 2\pi\int_B \mathrm{d}x\sqrt{|E^1|((E^2)^2 + (E^3)^2)}. \tag{94}$$

We can now see that in all the sectors with $k \neq 1$ the volume vanishes because then $E^2 = E^3 = 0$. All these degenerate sectors have to be rejected on physical grounds and we arrive at a unique sector of invariant connections given by the parameter $k = 1$.

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