Quantum cosmology: effective theory

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Abstract
Quantum cosmology has traditionally been studied at the level of symmetry-reduced minisuperspace models, analyzing the behavior of wave functions. However, in the absence of a complete full setting of quantum gravity and detailed knowledge of specific properties of quantum states, it remained difficult to make testable predictions. For quantum cosmology to be part of empirical science, it must allow for a systematic framework in which corrections to well-tested classical equations can be derived, with any ambiguities and ignorance sufficiently parameterized. As in particle and condensed-matter physics, a successful viewpoint is one of effective theories, adapted to specific issues one encounters in quantum cosmology. This review presents such an effective framework of quantum cosmology, taking into account, among other things, space-time structures, covariance, the problem of time and the anomaly issue.

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1. Introduction

If quantum cosmology is ever to be part of empirical science, it must be described by a good effective theory. There is no hope of exactly solving its equations in realistic models or to tame conceptual quantum issues made even more severe in the context of cosmology. The derivation of testable predictions requires systematic approximations at semiclassical order and beyond, and by experience with other areas of physics, effective actions or equations are the best available tools.

While the speculative part of quantum cosmology, addressing for instance the Planck regime or the status of multiverses, requires all subtleties of quantum physics to be considered—such as choices of Hilbert spaces, self-adjointness properties of Hamiltonians or unitarity of evolution, an understanding of deep conceptual issues and the measurement problem—physics can and must proceed without all these problems being solved\(^1\). Compare this situation for instance with quantum field theory, for which no rigorous interacting and non-integrable version is known. And yet, at the effective level it is the key tool behind the success of elementary particle physics. Given the immensity of the Planck scale, potentially observable effects in quantum cosmology are realized at low energies where semiclassical quantum gravity, with the first few orders in \(\hbar\) taken into account, suffices. This feature makes effective theory in quantum gravity and cosmology even more powerful than in other settings [1, 2]. As we will see in the course of this review, somewhat surprisingly, even conceptual problems of quantum gravity can advantageously be addressed with effective methods, especially with an extension to effective constraints.

Given the amount of research on effective theories and their applications, one may think that deriving an effective theory of quantum cosmology is a simple and well-understood problem. However, this is not at all the case. Quite general and powerful techniques of effective actions or potentials do exist, employed with great success in particle physics and condensed-matter physics alike. Quantum cosmology, on the other hand, is unique by virtue of several features. It requires aspects of effective equations not encountered in other fields, related for instance to the prevalence of canonical methods, the generally covariant setting lacking evolution by a unique time parameter, or the absence or inapplicability of non-perturbative ground states or other distinguished classes of states. These technical problems will be discussed in due course. For now, as a motivation of our detailed look into effective

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\(^1\) Especially in the loop-quantum-gravity community with its long and proud history of mathematical-physics primacy, it is sometimes said that one must become ‘less rigorous’ in order to find useful and interesting physical results. This statement is, of course, incorrect; one does not become a physicist by being a mathematician first and then turning a little less rigorous. Physics requires as much rigor as mathematics, but a different kind of rigor.
theory, we state the following two general problems by which quantum cosmology differs from other fields.

First, quantum cosmology is much like condensed-matter physics, with microscopic quantum degrees of freedom manifesting themselves on length scales far larger than their own. While the precise nature of microscopic degrees of freedom (strings, loops, . . . ) remains unclear and disputed among the different approaches, their presence in some form is widely agreed upon. By considering large structures or space-time regions made from many building blocks, quantum cosmology differs significantly from most situations encountered in elementary-particle physics, where events with a comparatively small number of particles in excited states close to the vacuum are studied. Quantum cosmology is a many-body problem, a situation in which it is difficult to derive and justify valid effective descriptions. The effective view has been put to good use in condensed-matter physics, but only thanks to rich and merciless experimental input to weed out wrong ideas and stimulate new successful ones. Quantum cosmology is not (yet?) subject to experimental pressure, and many (good and bad) ideas are sprouting. Effective cosmological theory must be able to stand on its own, requiring a systematic and rigorous formulation taking into account all features and consistency conditions to be imposed in quantum gravity.

As the second problem, we observe that the theoretical foundation of quantum cosmology is much weaker than that of condensed-matter physics to which it is otherwise quite close. We know well which Hamiltonian we should use to find all states and energies of excitations in a crystal, but mathematically the problem is challenging and calls for the approximations of effective theory. In quantum cosmology, we don’t even know which precise Hamiltonian or other underlying object to use for the dynamics of a universe. Even if we choose one particular approach to quantum gravity, its mathematical objects or its specializations to cosmology are incompletely known or understood, opening wide the door for ambiguities and spurious constructions.

We need a well-understood theory to pinpoint places where best to look for observational effects, and we need observations to guide our theoretical constructions. Quantum cosmology, with an incompletely understood theory and no current observations, is a slippery subject, depriving us of a good handle to grasp its implications. In the absence of experiments, we can only rely on conceptual arguments and internal mathematical consistency conditions which, however, come along with their own problems. In this situation, effective techniques have proven to be one of the few reliable approaches for physical evaluations of the theory, allowing one to include all crucial quantum effects in equations with clear physical meaning, and to take into account ambiguities by sufficiently general parameterizations. This general framework and its current status in the context of quantum cosmology are the topics of this review2.

2 Fundamental issues of quantum cosmology are reviewed in the companion article [3].
research on quantum cosmology and even quantum gravity, owing to their complicated nature. This intentional oversight implies a large number of ambiguities, fixed in those contexts only by ad hoc constructions. To keep this review focused, we will not discuss the rather large body of works in such directions, for instance those crucially using the distinction of a time variable by gauge-fixing or deparameterization in canonical settings, and only mention shortcomings in contexts in which they become apparent. Generally speaking, results derived with a distinguished choice of time (or gauge) cannot be considered physically reliable unless one can make sure that they do not depend on one’s choice of time.

In this section, we will discuss the main features that an effective theory of quantum cosmology must deal with, which includes covariance and state properties. The former ensures independence of choices of time, the latter deals with additional freedom in quantum theories. By these considerations, we will be guided toward suitable ingredients for the mathematical formulation of effective theory.

2.1. Covariance

Effective equations of quantum cosmology are supposed to modify some cosmological version of Einstein’s equation by quantum corrections. In most cases, such a cosmological version is a reduction to isotropic Friedmann–Lemaître–Robertson–Walker space-times or homogeneous Bianchi models (minisuperspaces), a restriction to some specific form of inhomogeneous degrees of freedom such as Lemaître–Tolman–Bondi or Gowdy geometries (midisuperspaces), or an inclusion of unrestricted but perturbative inhomogeneity around a background in the former classes of models.

2.1.1. Homogeneous models and automatic consistency. In homogeneous models, the dynamics is completely determined by one equation for gravitational degrees of freedom (such as the Friedmann equation) and one for matter (such as the continuity equation). The Friedmann equation of isotropic models,

\[
\left( \frac{\dot{a}}{a} \right)^2 + \frac{k}{a^2} = \frac{8\pi G}{3} \rho, \tag{1}
\]

depends only on first-order derivatives and is therefore a constraint, to be satisfied by initial values of second-order equations of motion. When interpreted as a constraint (the Hamiltonian constraint), it is usually written in the form of an energy-balance law:

\[
H := -\frac{3}{8\pi G}(\dot{a}^2a + ka) + E_{\text{matter}} = 0 \tag{2}
\]

with the matter energy \( E_{\text{matter}} = \rho a^3 \) contained in some region of unit coordinate volume. (See [4] for a detailed discussion of coordinate factors when the volume is not fixed, especially in the context of quantization.) In this form, the Hamiltonian constraint of gravity is obtained by varying the action by the lapse function \( N = \sqrt{-g_{00}} \). (For more on constraints and canonical gravity, see [5].)

Given the Friedmann equation and the continuity equation

\[
\dot{\rho} + 3 \frac{\dot{a}}{a} (\rho + P) = 0, \tag{3}
\]

with pressure \( P \), one can derive a second-order equation of motion by taking a time derivative of (1) and eliminating \( \dot{\rho} \): the Raychaudhuri equation

\[
\frac{\ddot{a}}{a} = -\frac{4\pi G}{3} (\rho + 3P). \tag{4}
\]
At this stage, we have all equations expected from the components of the isotropic Einstein tensor: the time-time component providing the Friedmann equation, the (identical) diagonal components of the spatial part amounting to the Raychaudhuri equation, and all off-diagonal components vanishing identically. The equations obtained are automatically consistent with each other: by construction, the time derivative of the Friedmann equation vanishes if the Raychaudhuri equation holds. Therefore, if the constraint imposed by the Friedmann equation holds for initial values at some time, it holds at all times.

This latter property is realized for a large class of systems describing versions of isotropic (or homogeneous) cosmology, not just for the classical one resulting from Einstein’s equation. As a phase-space function, $H(a, p_a)$ in (2), with the momentum $p_a = -3(4\pi G)^{-1}a\dot{a}$ as it follows from the variation $\partial L_{\text{grav}}^a / \partial \dot{a}$ of the Einstein–Hilbert action reduced to isotropy, plays the role of the Hamiltonian generating all equations of motion in proper time. The Raychaudhuri equation indeed follows from the Hamiltonian equations of motion $\dot{a} = \partial H / \partial p_a = \{a, H\}$ and $p_a = -\partial H / \partial a = \{p_a, H\}$ (the first of which is identical to the definition of the momentum $p_a$). The matter terms $\rho$ and $P$ are realized by

$$\rho = \frac{E_{\text{matter}}}{a^3}, \quad P = -\frac{1}{3a^2} \frac{\partial E_{\text{matter}}}{\partial a},$$

the negative change of energy by volume change. Matter equations of motion follow once $E_{\text{matter}}$ in (2) is expressed in terms of canonical degrees of freedom.

The phase-space function $H(a, p_a)$ itself evolves according to the same Hamiltonian law, $\dot{H}(a, p_a) = \{H(a, p_a), H\} = 0$ and is automatically constant in time, no matter what form $H(a, p_a)$ has. In homogeneous situations, the single Hamiltonian constraint that determines evolution is automatically preserved and consistent with evolution equations. We can easily modify $H$ by any form of quantum corrections without encountering consistency problems, issuing a powerful license to cosmological model builders.

Consistency remains valid when we consider different choices of time. So far, the equations were in proper time $\tau$. All other choices $t$ in homogeneous models are related to $\tau$ by $\tau(t) = \int N(t') \, dt'$, with a lapse function $N$ that enters Hamiltonian equations as well: if $d f(a, p_a)/d\tau = \{f, H\}$, we have

$$\frac{d f(a, p_a)}{d\tau} = \frac{d r}{d\tau} \frac{d f(a, p_a)}{d t} = N[f, H] \approx \{f, NH\}$$

for any other time with $d r/d\tau = N$. In the last step, we are allowed to pull the lapse function $N$ inside the Poisson bracket, keeping the equality satisfied as a ‘weak’ one, one that is valid provided the constraint $H = 0$ holds. Applying the general law to the constraint itself, we again observe consistency: $dH/dt = \{H, NH\} \approx 0$.

The Hamiltonian constraint generates not only evolution with respect to a given time choice, but also the transition between different choices as a gauge transformation. Infinitesimally, with $N$ close to one, we have $\tau = t + \epsilon$ with $\epsilon = \int (N - 1) \, dt$, and for any function $f$,

$$\delta f = f(\tau) - f(t) = \epsilon \frac{df}{d\tau} = \epsilon \{f, H\} \approx \{f, \epsilon H\}. \quad (6)$$

The Friedmann equation, amounting to the Hamiltonian constraint, is automatically invariant under changes of time, and so are its solutions. Also the evolution equations are invariant if we use the Jacobi identity for Poisson brackets:

$$\left\{ \frac{df}{dt}, \epsilon H \right\} = \{(f, NH), \epsilon H\} = \{(f, \epsilon H), NH\} + \{f, \{(NH, \epsilon H)\} \}
= \frac{d(f, \epsilon H)}{d\tau} - \{f, (d \epsilon / dt)H\} + \{f, (\delta N)H\}.$$
Rearranging, we see that the gauge-transformed \( f \) evolves in agreement with the gauge-transformed \( df/dt \), with a correction taking into account a possible gauge transformation of \( N \) and time dependence of \( \epsilon \).

The presence of a single Hamiltonian constraint therefore ensures dynamical consistency and invariance, even if quantum modifications occur. For this reason, homogeneous minisuperspace models are a simple and popular tool to investigate possible consequences of quantum gravity and cosmology. But for the very same reason, extreme care must be exercised when such models are used for physical predictions: the trivialization of consistency conditions does not hold in a more general context, and therefore spurious results can easily be produced in their absence.

2.1.2. Inhomogeneity and covariance. Compared with minisuperspace models, inhomogeneous cosmology presents a very different situation regarding consistency, even if inhomogeneity is small and treated perturbatively. For gravity and matter to fit together in Einstein’s equation or a quantum modification thereof, a version of the contracted Bianchi identity must hold. But this identity, relating different types of dynamical equations, is easily destroyed if quantum corrections, for instance those found in minisuperspace models, are inserted blindly. When amending inhomogeneous equations by quantum corrections, one must face the problem of anomaly freedom or covariance. Certain relations between different dynamical equations and gauge generators, classically implemented by the contracted Bianchi identity, must be preserved in the presence of quantum corrections.

This well-known classical fact is often overlooked in quantum treatments, especially those making use of gauge fixing or deparameterization. Gauge generators disappear when the gauge is fixed. A simple but illegitimate way out of difficult consistency problems is therefore to fix the gauge before quantum corrections are inserted. However, one then dispenses with ways to check consistency and cannot be sure that results obtained are physically viable. Most cases in which cosmological perturbations have been computed by gauge fixing in loop quantum cosmology, for instance, have by now been shown to be incorrect; important effects such as signature change have been overlooked. See also the instructive discussion of [6] in this context. We will come back to this issue later and for now continue with a classical discussion to provide more details.

The first implication of the Bianchi identity is the presence of constraints. If we write \( \nabla_\alpha G^\alpha_\mu = 0 \) in the form

\[
\partial_0 G^0_\mu = -\partial_\alpha G^\alpha_\mu - \Gamma^\alpha_{\nu\beta} G^\nu_\beta + \Gamma^\nu_{\nu\mu} G^\nu_\alpha,
\]

with spatial indices ‘\( \alpha \)’, it becomes evident that the components \( G^0_\mu \) of the Einstein tensor cannot contain second-order time derivatives: on the right-hand side, all factors in the three terms are at most second order in time, and there is one explicit time derivative on the left-hand side, leaving only the option of first time derivatives in \( G^0_\mu \). These components of the Einstein tensor (minus \( 8\pi G \) times the corresponding stress-energy components \( T^0_\mu \) if there is matter) are constraints on initial values, while the remaining components provide evolution equations.

In contrast to minisuperspace models, we are dealing with a larger constrained system of four independent and functional constraints, the Hamiltonian constraint \( H = G^0_0 - N^\alpha G^0_\alpha \) and the diffeomorphism constraint \( D = NG^0_\alpha \), which are to be imposed pointwise or for all possible multiplier functions \( N \) and \( N^\alpha \) in

\[
H[N] = -\int d^3x N(G^0_0 - N^\alpha G^0_\alpha) \quad \text{and} \quad D[N^\alpha] = -\int d^3x N^\alpha NG^0_\alpha.
\]

We are dealing with an infinite number of constraints. (To define these integrations, one introduces a foliation of space-time into spatial surfaces \( t = \text{const} \), also used to set up
canonical variables. The time direction \( t^a \) at each point, used to define time derivatives in evolution equations, may be different from the normal direction \( n^a \) to spatial slices in space-time, a freedom parameterized as \( t^a = N n^a + N^a \) with the lapse function \( N \) and the shift vector field \( N^a \). The linear combinations of \( G^a_\mu \) and \( \tilde{G}^a_\mu \) in (8), depending on the shift \( N^a \) and lapse \( N \), take into account that constraints refer to directions normal and tangential to spatial slices, not to coordinate directions such as the zero-index of the Einstein tensor for a component along the time-evolution vector field \( t^a \).)

As before, for consistency the constraints must always hold provided they are imposed for initial values, a feature that is guaranteed by the Bianchi identity as well. If we combine the Einstein tensor and the stress-energy tensor \( T_{\mu\nu} \) of matter in (7), we see that \( \delta_\pi (G^a_\mu - 8\pi GT^a_\mu) \) vanishes at any time provided the constraints \( G^a_\mu - 8\pi GT^a_\mu \) themselves (and therefore their spatial derivatives) vanish at that time and the evolution equations hold. By virtue of the contracted Bianchi identity, the constraints are consistent with evolution. Finally, as a third consequence, we see that all equations, Einstein’s equation and the contracted Bianchi identity as a consistency condition, are covariant and independent of coordinates used. Therefore, solutions will be covariant. All equations hold irrespective of the choice of coordinates, a well-known feature in perturbative cosmology which allows one to express all equations explicitly in terms of gauge-invariant variables [7, 8].

As in our discussion of minisuperspace models, a canonical view is useful to analyze which consistency conditions are satisfied automatically and which ones are non-trivial. There is a Hamiltonian constraint, and therefore Hamiltonian equations \( \dot{f} = \{f, H\} \) are generated by a constraint \( C \). However, in the inhomogeneous context, the constraint is not unique (up to a pre-factor \( N \)), nor is time evolution. We have a much larger choice of possible time variables to generate evolution. The most general version of equations of motion is obtained if we use all our constraints in a linear combination, defining \( H(N, N^a) := H[N] + D[N^a] \). For fixed \( N \) and \( N^a \), the Hamiltonian flow \( \dot{f} = \{f, H[N, N^a]\} \) is then equivalent to Lie derivatives \( \dot{f} = \mathcal{L}_f; f \) along the time-evolution vector field \( t^a = N n^a + N^a \) in space-time, foliated by spatial slices with unit normals \( n^a \).

For all constraints to be preserved by the evolution equations they generate, we need \( \{H[M, M^a], H[N, N^a]\} \approx 0 \) for all \( M, N, M^a \) and \( N^a \). If this condition is satisfied, the constraints are said to form a first-class system. Unlike in homogeneous models, where \( H[M] \) always commutes weakly with \( H[N] \), the general condition is highly non-trivial and provides strong restrictions on consistent modifications of Einstein’s equation. Quantum corrections can no longer be inserted at will.

The same conditions that generate evolution provide gauge transformations, classically equivalent to coordinate changes. We use the same general combination as before, \( H[\epsilon, \epsilon^a] \), but interpret the multipliers \( \epsilon \) and \( \epsilon^a \) differently, not related to a time-evolution vector field. Instead, the gauge transformation \( \delta_\epsilon f = \{f, H[\epsilon] + D[\epsilon^a]\} \) with the classical constraints is equivalent to a coordinate transformation or the Lie derivative \( \mathcal{L}_\epsilon f \) along the time-evolution vector field \( \dot{\xi}^a \) with components such that \( \epsilon = N\dot{\xi}^0 \) and \( \epsilon^a = \dot{\xi}^a + N^a\xi^0 \) [9]. The factors of \( N \) and \( N^a \) again result because space-time coordinate changes and the components of \( \dot{\xi}^a \) refer to coordinate directions, while constraints refer to directions normal and tangential to spatial slices with normal \( n^a = N^{-1}(t^a - N^a) \). Also regarding gauge invariance, the condition of a first-class constraint algebra is then sufficient for consistency: in this case, all constraints are gauge invariant, \( \delta_\epsilon [H[N, N^a]] = [H[N, N^a], H[\epsilon, \epsilon^a]] \approx 0 \), and so are the evolution equations they generate. With this full set of gauge transformations, one can freely change the constant-time spatial surfaces used to define canonical variables and to integrate the constraints (8). We are then dealing with a covariant theory of space-time, not just with a theory on a fixed spatial foliation.
2.1.3. Hypersurface-deformation algebra. The crucial consistency condition for any classical constrained system, its quantization, or an effective theory thereof, is therefore that it be first class: all constraints $H[N, Na]$ must have Poisson brackets that vanish when the constraints are imposed,

$$[H[M, Ma], H[N, Na]] \approx 0.$$  \hspace{1cm} (9)

For gravity, or any generally covariant space-time theory, the specific form is the hypersurface-deformation algebra [10]

$$[D[Ma], D[Na]] = D[LNb Ma],$$  \hspace{1cm} (10)

$$[H[M], D[Na]] = H[LNb M],$$  \hspace{1cm} (11)

$$[H[M], H[N]] = D[qab(M \nabla bN − N \nabla bM)]$$  \hspace{1cm} (12)

with the spatial metric $qab$.

For a consistent quantization, an algebra of this form must be realized with commutators for constraint operators instead of Poisson brackets, and an effective constrained system must have quantum-corrected constraints such that a first-class algebra holds with Poisson brackets. If this is realized, no gauge transformations are broken by quantization and the quantum or effective theory is called anomaly-free. If this condition is satisfied, all consistency conditions that are classically implied by the contracted Bianchi identity hold in the presence of quantum corrections, and the (quantum) theory describes space-time rather than just a family of spatial slices. This property may be achieved with exactly the same form of the algebra, or with one that shows quantum corrections not just in the constraints but also in the structure functions of the algebra, as long as two constraints still commute up to another constraint. One universal example found in loop quantum gravity, as the most prominent result regarding hypersurface deformations with quantum corrections, has (10) and (11) unchanged, but (12) modified to [11]

$$[H[M], H[N]] = D[\beta q^{ab}(M \nabla bN − N \nabla bM)]$$  \hspace{1cm} (13)

with some phase-space function $\beta$. If the classical hypersurface-deformation algebra is modified, gauge transformations no longer correspond to Lie derivatives by space-time vector fields. Not just the dynamics but even the structure of space-time may be modified by quantum effects. We will discuss specific examples and results in later parts of this review.

By analyzing quantum or effective constraints and their algebra, one can draw conclusions about quantum space-time structures. For instance, once the full hypersurface-deformation algebra is known, one can specialize it to Poincaré transformations by using linear $N$ and $Na$.

With $N(x) = \Delta t + \nu x$, for instance, we have a combination of a time translation by $\Delta t$ and a boost by $\nu$. With $\beta \neq 1$ in (13), the usual Poincaré relations are modified. Although this may look like a version of deformed special relativity [12–14], there is no direct relation: in deformed special relativity, one has non-linear realizations of the Poincaré algebra, with structure constants depending on the algebra generators. In (13), we have corrections of structure functions depending on phase-space degrees of freedom, not directly on the algebra generators $H[N]$ and $D[Na]$. A deformed version of special relativity would require a relation between phase-space variables, such as extrinsic curvature, and some space-time generators, such as energy. Relations of this form do exist in some regimes, for instance in asymptotically flat ones using the ADM energy, but not in general.

2.1.4. Consistent and inconsistent quantum cosmology. In general terms, the problem of canonical quantum cosmology can be formulated as follows: find quantum corrections
in $H[N, N^a]$, perhaps motivated by some full theory of quantum gravity, such that these constraints remain first class. This statement presents a well-defined mathematical problem of classifying deformed algebras. For every consistent version that may exist, we can compute and analyze equations of motion by standard means, as explicitly written out above in the general classical case. At the present stage, several examples of consistent deformations of constraints remaining first class are known, mainly from loop quantum gravity, but there is no general classification of these infinite-dimensional algebras.

As already mentioned, there are attempts to shortcut through the difficult calculation of these algebraic structures by fixing the gauge before quantum corrections or other modifications are put in. If the gauge is fixed, one would no longer consider $H[\epsilon, \epsilon^a]$ as gauge generators, but only use $H[N, N^a]$ as constraints and to generate evolution. Some consistency conditions still need to be satisfied because the constraints are to be preserved by evolution, but this can usually be achieved more easily than in the non-gauge fixed case in which more fields are present. However, even if formally consistent versions of preserved constraints can be found in this way, such as those in [15], they are not guaranteed to be consistent because only a subclass of the constraint algebra can be tested when some modes are eliminated beforehand. Even if these are classical gauge modes, some consistency conditions and physical effects are overlooked. Moreover, the procedure is intrinsically inconsistent because one would first fix the gauge as it is determined by the classical constraints, and then proceed to modify the constraints that generate the gauge.

A consistent scheme could be obtained only when the modified gauge structure is taken into account from the very beginning, but for that one would have to know a consistent version of non-gauge fixed constraints, not just of the gauge-fixed ones. Finally, having fixed the gauge, there is no way of calculating general gauge-invariant observables. Also here, one could only refer to the classical invariant variables, whose form however must be modified when quantum corrections are put into the constraints. Note that quantum space-time structures and modified constraints in most cases imply departures from classical manifold pictures, as we will see explicitly in the examples provided later. One can no longer refer to the usual form of coordinate transformations to compute gauge-invariant variables without using the constraints explicitly. In modified space-times, the constraints are the only means to compute gauge flows and invariants, but this can be done only if the gauge has not been fixed.

Algebraic conditions can be simplified even more when gauge fixing is combined with deparameterization. With the latter procedure, one chooses a phase-space degree of freedom, for instance from matter, to rewrite constraint equations as relational evolution equations with respect to this variable. Not just gauge transformations but even constraints then disappear from the system, and no strong consistency conditions remain. A popular example is the coupling of a free, massless scalar field $\phi$, whose homogeneous mode $\bar{\phi}$ in an expansion $\phi = \bar{\phi} + \delta \phi$ around some background can be treated as a global time function. The canonical scalar Hamiltonian

$$H_{\text{scalar}} = \frac{1}{2} \int d^3 x \left( \frac{p^2_{\phi}}{\sqrt{\det q}} + \sqrt{\det q} q^{ab} (\partial_a \phi)(\partial_b \phi) \right)$$

$$= \frac{1}{2} \left( \frac{\bar{p}_{\phi}^2}{\sqrt{\det q}} + \int d^3 x (\cdots) \right)$$

with the momentum $p_{\phi} = \bar{p}_{\phi} + \delta p_{\phi}$ then has a purely kinetic background term and is completely independent of $\phi$. The momentum $\bar{p}_{\phi}$ is therefore a constant of motion and never becomes zero unless it vanishes identically. The background scalar $\bar{\phi}$ has no turning points and is monotonic, serving as a global internal time along classical trajectories.
The Hamiltonian generating evolution with respect to this variable is obtained by solving the Hamiltonian constraint $H_{\text{gravity}} + H_{\text{scalar}} = 0$ (with fixed $N$ as part of the gauge choice) for $\tilde{p}_\phi = H_\phi(q_{ab}, p^{ab}, \delta \phi, \delta p_\phi)$: we have $\dot{\phi} = \{\phi, H_\phi\} = 1$ and $\dot{\tilde{p}}_\phi = \{\tilde{p}_\phi, H_\phi\} = 0$, consistent with evolution with respect to $\tilde{\phi}$ where the dot stands for $d/d\tilde{\phi}$, as well as Hamiltonian equations for the remaining variables, such as $\dot{q}_{ab} = \{q_{ab}, H_\phi\}$ and $\delta \phi = \{\delta \phi, H_\phi\}$. There is just one Hamiltonian generating all evolution equations, instead of a set of infinitely many constraints. Almost as in minisuperspace models one can then implement in $H_\phi$ any quantum corrections one may desire. (In the context of cosmology, this approach has been suggested for instance in [16] in an analysis of Gowdy models and possible quantizations.)

Deparameterization is a powerful mathematical tool to derive properties of physical Hilbert spaces, for which no general method exists in the absence of deparameterizability. (See also section 4.1.5.) In quantum cosmology, this method has been applied in [17], and used recently to derive several aspects of self-adjointness and unitarity of evolution [18–20]. But it cannot serve as a valid procedure to evade the anomaly problem and do physical evaluations. To start with, most realistic systems are not globally deparameterizable, with one variable having no turning points at all. Moreover, also this procedure, on its own, cannot weed out physical inconsistencies in spite of its formal consistency. One has the same drawbacks as in the gauge-fixed approach, and on top of that one has distinguished (or even introduced) one degree of freedom as time. For physical consistency, one should then show that results for observables do not depend on one’s choice of time after quantization, but no systematic procedures exist to this end, constituting part of the problem of time in quantum gravity [21–23]. (See [24] for a discussion in the context of deparameterization or reduced phase-space quantization.) And even if one thinks that the distinguished time $\tilde{\phi}$ should be sufficient for all physical purposes and does not worry about relating results in different times, the fact that there is no analog of the Bianchi identity to constrain modifications should arouse suspicion.

Gauge fixing and deparameterization are not necessarily bad, but they provide reliable results only when they are used after a consistent version of quantum-corrected constraints has been found. When this is the case, it is clear that all equations are consistent and gauge covariant, and instead of computing complete gauge-invariant variables for the corrected constraints, one may well pick a gauge or choose an internal time and work out physical implications. There is also a possibility of providing consistent results with gauge fixing or deparameterization before quantization, but then one would have to show that all possible gauge fixings or deparameterizations would lead to the same physical observables. This requirement can be achieved in cases of simple constraints, such as the Gauss constraint of gravity in triad or connection variables as described at the end of section 5.1, but presents a much more involved problem for the complicated Hamiltonian constraint. Problems and physical inconsistencies arise always when the gauge or time is chosen according to the classical system, and modifications of the constraints and thereby gauge transformations are inserted later.

2.2. States

Covariance or analogs of the contracted Bianchi identity severely constrain consistent versions of quantum corrections, raising the manifold and metric structures underlying space-time in general relativity to the effective or quantum level. Although space-time structures and their covariance principles may then differ significantly from well-known classical ones, there is still a consistent dynamical theory independent of coordinates and gauge choices, and the set of all equations has meaningful solutions available for well-defined predictions. In addition
to these restrictions on quantum corrections based on gauge aspects, the quantum theory of gravitational degrees of freedom should tell us what form of modifications we can have.

2.2.1. Moments. Effective equations, in general terms, describe quantum evolution by a smaller, more manageable number of degrees of freedom compared with the full quantum theory considered. When we go from classical physics to quantum physics, every degree of freedom we have at first is replaced by infinitely many parameters, for instance values the whole wave function takes at all points in configuration space. It is difficult to deal with values of wave functions in physical terms. Another parameterization, more convenient for effective whole wave function takes at all points in configuration space. It is difficult to deal with values of wave functions in physical terms. Another parameterization, more convenient for effective whole wave function takes at all points in configuration space. It is difficult to deal with values of wave functions in physical terms. Another parameterization, more convenient for effective whole wave function takes at all points in configuration space. 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It is difficult to deal with values of wave functions in physical terms.

Effective solutions, describing the evolution of a quantum state, depend not only on classical variables but also on the quantum state
used, specified for instance by initial values of its moments. In quantum cosmology, one first promotes the constraint (2) expressed in canonical variables $a$ and $p_a$ as

$$H(a, p_a) = -\frac{2\pi G}{3} \frac{p_a^2}{a} + E_{\text{matter}}$$

(19)

to an operator $\hat{H}$, choosing some ordering of $\hat{a}$ and $\hat{p}_a$. Dirac quantization then implements the classical constraint equation $H(a, p_a) = 0$ by the condition $\hat{H}\langle\psi\rangle = 0$ on physical states. In particular, the expectation value $\langle\hat{H}\rangle$ must vanish in all physical states. If we express this equation as a functional equation on the space of expectation values and moments parameterizing states, we obtain an expression such as

$$\langle\hat{H}\rangle = -\frac{2\pi G}{3} \left( \frac{\langle\hat{p}_a\rangle^2}{\langle\hat{a}\rangle} + \frac{(\Delta_{\hat{p}_a})^2}{\langle\hat{a}\rangle} + \cdots \right) + \langle\hat{E}_{\text{matter}}\rangle$$

(20)

where we have used $\langle\hat{p}_a^2\rangle = \langle\hat{p}_a\rangle^2 + (\Delta_{\hat{p}_a})^2$ and the dots indicate additional terms that contain the covariance of $a$ and $p_a$ as well as higher moments, and depend on the specific ordering chosen. If we take into account only expectation values in $\langle\hat{H}\rangle = 0$, the classical Hamiltonian and the classical constraint surface are obtained. With fluctuations and higher moments, quantum corrections result that couple moments to expectation values and change the classical constraint surface. A systematic derivation and analysis of such moment terms, starting with expectation values of Hamiltonians and constraints, is the key ingredient of effective theories.

The moments couple to expectation values, thereby providing quantum corrections to the classical motion, and their values therefore enter effective equations. A complete effective theory cannot leave the moments in equations as unknowns and instead provides evolution equations or other conditions for them as well. But some freedom always remains, for instance in the initial values chosen for evolution equations of moments. If effective theories are formulated for expectation values without including additional degrees of freedom such as moments to describe the evolution of classes of states, the specific states must either be restricted to provide unique effective equations, or be parameterized for a more general set. Often, such a state dependence enters effective theories only implicitly, for instance in the unique-looking low-energy effective action [26] free of any state parameters. This effective action describes low-energy effects of states near the vacuum of the interacting theory. In this way, the class of states is specified, certainly a rather small set compared to all possible states.

In quantum cosmology, we are often interested in high-energy, Planckian phenomena and cannot restrict attention to the low-energy effective action. Even in low-energy regimes, which would be all we need to make contact with potential observations, it is not clear what low-energy state should be used. Quantum cosmology in its non-perturbative form, or quantum gravity in general, does not have a vacuum or other distinguished low-energy state. Effective theories of quantum cosmology must therefore be more general than the low-energy effective action, leaving more freedom for states parameterized in some suitable way.

Even if we restrict attention to semiclassical regimes, the class of states to be considered may be large: simple Gaussians provide at most a two-parameter family within a large set of semiclassical states when they are fully squeezed. For uncorrelated Gaussians, wave functions

$$\psi_\sigma(a) = N \exp\left(-\frac{(a - \langle\hat{a}\rangle)^2}{4\sigma^2}\right) \exp(-ia\langle\hat{p}_a\rangle/\hbar)$$

(21)

with a normalization constant $N$, we have, besides the two expectation values $\langle\hat{a}\rangle$ and $\langle\hat{p}_a\rangle$ on which the state is peaked, only one quantum parameter, the variance $\sigma$. The most general Gaussian state is of the form $\psi(z)(a) = \exp(-z_1a^2 + z_2a + z_3)$ with three complex numbers $z_i$ such that $\text{Re} z_1 > 0$ for normalizability. Out of these six real parameters, the two contained in
$z_3$ do not matter for moments because the real part is fixed by normalization and the imaginary part contributes only a phase factor. For the remaining parameters, writing $z_1 = \alpha_1 + i\beta_1$ and $z_2 = \alpha_2 + i\beta_2$ with real $\alpha_i$ and $\beta_i$, we compute expectation values

$$\langle \hat{a} \rangle = \frac{\alpha_2}{2\alpha_1}, \quad \langle \hat{p}_a \rangle = \hbar \frac{\alpha_1 \beta_2 - \alpha_2 \beta_1}{\alpha_1}$$

(22)

and second-order moments

$$(\Delta a)^2 = \frac{1}{4\alpha_1}, \quad (\Delta p_a)^2 = \hbar^2 \alpha_1 + \hbar^2 \frac{\beta_1^2}{\alpha_1}, \quad \Delta (ap_a) = -\hbar \frac{\beta_1}{2\alpha_1}.$$  (23)

One easily confirms that the uncertainty relation (18) is always saturated.

Deviations from saturation are much more difficult to parameterize, but easily occur for evolved semiclassical states even if they start out as a Gaussian. And even if one stays close to the saturation condition and does not vary second-order moments much beyond the values they can take for Gaussians, a Gaussian determines all higher moments in terms of the real and imaginary parts of $z_1$. Our general semiclassicality condition $(\Delta a \Delta p_a) \sim O(\hbar^{(b+c)/2})$ provides an infinite-parameter family instead of the special 2-parameter one realized for Gaussians. Unless one can motivate Gaussians by other means, for instance proximity to the Gaussian harmonic-oscillator ground state or the vacuum of a free field theory, using them exclusively may easily be too restrictive. (Given the large parameter space of states, one may be tempted to refer to probabilistic arguments to pick ‘likely’ states, following ideas that go back to an analysis of inflation in quantum cosmology [27, 28]. However, such probability considerations, though popular, are difficult, if not impossible, to make sense of in quantum cosmology [29].)

Not just the absence of a vacuum state but several other special properties of quantum cosmology are important when we consider possible states.

- Quantum cosmology considers long-term evolution. Even if we may be able to choose a specific form of semiclassical states at large volume and small curvature, it may change much when states are evolved back to high densities to infer possible implications at the big bang.
- As already mentioned, even the form of semiclassical states is unclear. It is customary to explore semiclassical features using simple and nicely peaked Gaussian states. In quantum mechanics, such states provide interesting information, and they are realized in exactly this form as coherent states or the ground state of the harmonic oscillator. In quantum field theory, Gaussian states are then close to the perturbative vacuum even for interacting theories. The dynamics of quantum cosmology, however, is not near that of the harmonic oscillator (except for some special models), and the unquestioned use of Gaussians is more difficult to justify. But going beyond Gaussians is complicated in terms of wave functions, whose parameters then become much less controlled.
- It is not clear how precisely quantum cosmology can be derived from some full theory of quantum gravity, but the number of degrees of freedom is certainly reduced either by exact symmetries or by perturbing around some background. In such situations, when degrees of freedom are eliminated, pure states easily become mixed. For general evolution equations able to model a full state, we should therefore allow for the possibility of mixed states, again going beyond pure Gaussians or other specific wave functions. Moments provide a parameterization of mixed states as well since they are based only on the notion of expectation values.
- The question of covariance affects also the choice of classes of states. A state chosen in a minisuperspace model must have a chance of being the reduction of a full state that does not break covariance. This question may be difficult to analyze at the level of wave functions, but it also shows that a sufficiently large freedom in the choice of states must
be included in considerations that aim to provide a consistent formulation of quantum cosmology.

Since state properties are important for effective actions and quantum back-reaction, we should be as general as possible with the choice of states we consider. With wave functions or density matrices for mixed states, such a generality is difficult to achieve, but it is possible with parameterizations such as the one by moments. Moments provide a general form of semiclassical states, as already introduced. In effective theories, they are subject to their own evolution equations which show how they may change as high-density regimes are approached. They go well beyond the two-parameter family of squeezed Gaussians, and describe pure and mixed states alike.

2.2.3. Quantum phase space and covariance. Covariance at the level of effective equations with quantum back-reaction can be addressed by combining the moment parameterization with the methods of the previous section, deriving consistent constrained systems amended by quantum corrections that include the moments. For the last question, we must be able to fit moments into a phase-space structure, so as to be able to compute Poisson brackets such as \( \{ H[M, M^*], H[N, N^*] \} \) with constraints that may include moment terms, such as an inhomogeneous version of (20).

This construction is indeed possible: together with expectation values, the moments form a quantum phase space with Poisson brackets defined by the commutator [30], first for expectation values of arbitrary operators:

\[
\{ \langle \hat{A} \rangle, \langle \hat{B} \rangle \} = \frac{\{ [\hat{A}, \hat{B}] \}}{i\hbar}.
\] (24)

This bracket satisfies the Jacobi identity and is linear. If we extend it to polynomials of expectation values by imposing the Leibniz rule, all laws for a Poisson bracket are satisfied, and we can apply the definition to moments. For instance, we obtain \( \{ \langle \hat{a} \rangle, \langle \hat{p}_a \rangle \} = 1 \) and \( \{ \langle \hat{a} \rangle, \Delta(a^b p^c) \} = 0 = \{ \langle \hat{p}_a \rangle, \Delta(a^b p^c) \} \) for all \( b \) and \( c \). The moments, as defined here, are symplectically orthogonal to expectation values, a convenient feature for calculations. Poisson brackets between different moments have been computed explicitly but are lengthy; see [30] and the correction of a typo in [25]. For low orders, it is usually more convenient to compute Poisson brackets directly from the definition (24). For instance, we calculate

\[
\{ (\Delta q)^2, (\Delta p)^2 \} = \{ (\hat{q}^2) - \langle \hat{q} \rangle^2, (\hat{p}^2) - \langle \hat{p} \rangle^2 \} = \frac{\{ [\hat{q}^2, \hat{p}^2] \}}{i\hbar} - 2\langle \hat{p} \rangle \frac{\{ [\hat{q}^2, \hat{p}] \}}{i\hbar} - 2\langle \hat{q} \rangle \frac{\{ [\hat{q}, \hat{p}^2] \}}{i\hbar} + 4\langle \hat{q} \rangle \langle \hat{p} \rangle \frac{\{ [\hat{q}, \hat{p}] \}}{i\hbar}
\]

using the Leibniz identity and (24).

If we know how a state enters effective constraints via its moments, a question which we will address in due course, we can compute Poisson brackets of effective constraints and see whether they provide a consistent deformation of the classical constraint algebra. If a consistent deformation is realized, the system can be analyzed further by standard canonical means to arrive at observables and dynamical equations. Note, however, that the Poisson tensor for moments truncated to some order is in general not invertible, for instance on the three second-order moments which form an odd-dimensional Poisson manifold: with (25) and similar calculations for the other second-order moments, we obtain

\[
\{ (\Delta q)^2, (\Delta p)^2 \} = 4\Delta(qp),
\]

(26)

\[
\{ (\Delta q)^2, \Delta(qp) \} = 2(\Delta q)^2,
\]

(27)
the three-dimensional Poisson manifold of second-degree polynomials. Symplectic geometry therefore cannot be used for effective theories, while Poisson geometry is available from the definition (24). All relevant properties of constrained systems, such as the distinction between first and second class or properties of gauge transformations, can be formulated at the level of Poisson geometry [31].

2.2.4. Quantum-gravity states. In summary of this section, we note that there are several specific issues in the derivation of effective theories for quantum cosmology, compared to other fields in which such methods are in use. The central theme is covariance, an issue which can be addressed only if one goes beyond the traditional quantum-cosmological realm of minisuperspace models. The notion of covariance and the question whether it is realized consistently may be affected by new quantum space-time structures introduced by the specific form of quantum geometry in one’s approach to quantum gravity.

The second, less obvious source of potential modifications of covariance is the form of dynamical quantum states used. Effective actions or equations depend on the classes of quantum states whose evolution they approximate, which should be specific solutions of some underlying quantum theory of gravity. Even if a theory such as quantum gravity is covariant, the selection of specific solutions may always break this symmetry. Covariance may then be realized in a deformed way, or only partially within one effective theory. For instance, even if the states used are peaked on covariant classical fields, giving rise to covariant effective terms depending on expectation values, their fluctuations or higher moments may not be fully covariant. Changing the gauge in quantum gravity may then require the transition to a different effective theory, in which different state parameters have been used (reminiscent of the application of background-field methods in standard quantum field theory). On the other hand, if the class of states is sufficiently large, all gauge-related parameters could be encompassed within one effective theory. These considerations highlight the importance of the selection of states in the derivation of effective theories.

Both quantum geometry and quantum dynamics must be part of one consistent quantum theory of gravity; in a complete treatment, their effects therefore cannot be separated from each other. However, they are derived by different means, making use of different expansions of the expectation-value function \( \langle \hat{H} \rangle \) of the Hamiltonian or Hamiltonian constraint in the class of states used. In what follows, as in most derivations in the literature, we will split the treatment into one of quantum-geometry corrections first, as they are easier to see, followed by a discussion of quantum-dynamics corrections. When their expressions are known, we can compare implications of different effects and see if some are more relevant than others in specific regimes.

In the canonical setting, quantum-geometry corrections are specific to loop quantum gravity which has given rise to many results regarding background-independent quantization [32–34]. The effects in \( \langle \hat{H} \rangle \) are not unique, but characteristic enough to show implications for quantum space-time structure. After an overview of these terms in the next section, we will discuss dynamical quantum back-reaction, obtained from a further expansion of \( \langle \hat{H} \rangle \) by the moments parameterizing states. We will see the relation of canonical formulations to the low-energy effective action used in particle physics and the role of higher time derivatives in effective equations. Finally, we will put together our results to find properties of general effective actions taking into account all possible effects of canonical quantum gravity, and thereby shed light on quantum space-time structure.
3. Quantum geometry of space

Canonical gravity implements space-time structure by imposing the constraints $H[N] + D[N^a]$ and requiring invariance under the gauge flow they generate. (There may be additional constraints, such as the Gauss constraint if triad variables are used. Such constraints, however, restrict auxiliary degrees of freedom not related to transformations of space-time.) The diffeomorphism (and Gauss) constraint generates a simple flow by Lie derivatives, and has a direct action on quantum states. If we use states $\psi[q_{ab}]$ as in Wheeler–DeWitt quantum gravity (leaving aside the complicated question of how to define an inner product) we have a formal action

$$\hat{D}[N^a]\psi[q_{bc}] = \psi[L_{N^a}q_{bc}]$$

States are annihilated by the diffeomorphism constraint if they depend only on spatial invariants, of the same form as classically, and expectation values in non-invariant states transform according to the classical gauge transformations. In loop quantum gravity, the action on states is different because discrete spatial structures do not allow infinitesimal diffeomorphisms to be represented. But for finite diffeomorphisms, the situation is exactly as just described. Therefore, we do not expect significant quantum modifications of the spatial diffeomorphism constraint (but see section 3.2). Similarly, the Gauss constraint, if there is one, has a simple and direct action that does not suggest modifications; see also the end of section 5.1.

3.1. Hamiltonian constraint

The Hamiltonian constraint $\hat{H}[N]$ presents a different story. It cannot be quantized directly by promoting its (complicated) classical gauge flow to an action on states. The only procedure to arrive at a constraint operator is tedious: inserting basic operators quantizing the classical kinematical phase space into the expression for the Hamiltonian constraints. As a phase-space function, the constraint contains rather involved combinations of the basic fields, which require regularization and sometimes even other modifications for a well-defined operator to result [35, 36]. Also on general grounds, we do expect quantum corrections in the Hamiltonian constraint because it includes all about the dynamics of the theory. The theory being interacting, quantum corrections must result. The Hamiltonian constraint is therefore the place where we should look for characteristic quantum corrections of different theories, as well as possible restrictions by consistency requirements.

3.1.1. Gauge flow. A constraint operator $\hat{H}[N]$ restricts states by $\hat{H}[N]|\psi\rangle_{\text{phys}} = 0$ and generates a gauge flow $|\psi\rangle = \exp(-i\hat{H}[\epsilon]/\hbar)|\psi\rangle$. Physical states, on which $\exp(-i\hat{H}[\epsilon]/\hbar)$ acts as the identity, are gauge-invariant, and the gauge flow need not be considered separately if first-class constraint operators are solved. But exact solutions are complicated to find, and when quantum corrections are computed by systematic approximation schemes, the situation is quite different. Expectation values are constrained by $\langle \hat{H}[N] \rangle$, a weaker condition than $\hat{H}[N]|\psi\rangle = 0$. We have additional constraints $\langle (\hat{f} - \langle \hat{f} \rangle)\hat{H}[N] \rangle = 0$, an enlarged set of constraints which all vanish in physical states, for arbitrary $\hat{f}$. These constraints in general are all independent, constraining not just expectation values but also moments. In an effective theory, as spelled out in detail later, one solves this infinite set of quantum phase-space constraints order by order in the moments. To any given order, the sharp condition $\hat{H}[N]|\psi\rangle_{\text{phys}} = 0$ for physical states is not fully implemented, and on the corresponding solution space there is a non-trivial gauge flow by quantum constraints. Moreover, the effective treatment at this stage is more general because one does not assume a (kinematical) Hilbert-space structure when solving the constraints.
for moments; therefore the standard argument of a trivial gauge flow does not apply. At the effective level, there are non-trivial gauge transformations by quantum constraints, bringing solution procedures closer to classical ones: one solves phase-space constraints and factors out their gauge.

For an effective theory, the key ingredient is therefore the expectation value \( \langle \hat{H}[\epsilon] \rangle \) in a sufficiently large class of states, or the general expression parameterized by the moments of states. As in (20), moments then appear in quantum corrections that change the constraint surface. With a modified constraint surface, the gauge flows must receive quantum corrections as well for them to be tangential to the constraint surface mapping solutions to constraints into other solutions, as required for a first-class system. Indeed, the expectation value of the constraint, an expression that includes quantum corrections, determines the gauge flow on the quantum phase space with Poisson brackets (24) by

\[
\delta_\epsilon (\hat{O}) (\epsilon) = \epsilon \frac{\delta}{\delta \epsilon} \langle \psi | \exp(i \hat{H}[\epsilon]/\hbar) \hat{O} \exp(-i \hat{H}[\epsilon]/\hbar) | \psi \rangle = \frac{\{ [\hat{O}, \hat{H}[\epsilon]] \}}{\hbar} = \{ \langle \hat{O} \rangle, \langle \hat{H}[\epsilon] \rangle \}
\]

(29)

for expectation values \( \langle \hat{O} \rangle (\epsilon) = \epsilon \langle \psi | \hat{O} | \psi \rangle \), and therefore for any quantum phase-space function such as the moments by using the Leibniz rule. If the constraint surface changes by corrections in \( \hat{H} \), so do the gauge transformations. For the quantum corrected constraint surface and the gauge flow we are therefore required to compute \( \langle \hat{H}[\epsilon] \rangle \) in general kinematical states.

If quantum constraint operators are represented in an anomaly-free way, such that any commutator \([\hat{C}_1, \hat{C}_2]\) is an operator of the form \( f(q, p) \hat{C}_3 \) with another constraint operator \( \hat{C}_3 \) and structure functions \( f(q, p) \), the quantum constraints \( \langle \hat{C}_i \rangle \) form a consistent first-class system: \( \{ \langle \hat{C}_1 \rangle, \langle \hat{C}_2 \rangle \} = \{ [\hat{C}_1, \hat{C}_2] \} / i \hbar = \langle f(q, p) \hat{C}_3 \rangle \). Since all expressions such as \( \langle f(q, p) \hat{C}_3 \rangle \) vanish when computed in physical states, they provide effective constraints (in general independent of \( \langle \hat{C}_3 \rangle \) as phase-space functions). If all these constraints are imposed, the effective constrained system is first class and has a consistent gauge flow generated by all these constraints [37–39].

Such systems of infinitely many constraints for each local classical degree of freedom can be difficult to analyze. However, just as the moments obey a hierarchy in semiclassical regimes, the effective constraints can be truncated to finite sets to any given order in \( \hbar \) or in the moments. The leading corrections can be found in direct expectation values \( \langle \hat{C}_i \rangle \), restricting expectation values with quantum corrections that depend on the moments. For instance, (20), when imposed as a constraint, shows how the classical constraint surface and the gauge flow of \( \langle \hat{a} \rangle \) and \( \langle \hat{p}_a \rangle \) are changed by fluctuations \( \langle \Delta p_a \rangle^2 \). These corrections depend on the value of \( \langle \Delta p_a \rangle^2 \), which is constrained and subject to gauge flows by higher-order constraints such as \( \langle \hat{p}_a \hat{H} \rangle \). When all constraints have been solved and gauge flows factored out to a certain order, the condition \( \hat{H}[\psi] = 0 \) has been implemented for states used in expectation values and moments. One has then computed observables in physical states, sidestepping the complicated problem of computing an integral form of the physical inner product. This is one example for the use of effective methods to tame complicated technical and conceptual issues in quantum gravity. Even the problem of time can be solved, at least at the semiclassical level: different choices of time are related by mere gauge transformations in the quantum phase space [40–42]. We will come back to these conceptual question in section 4.1.5, and for now note the lesson that expectation values of constraints supply the key ingredient for effective gauge theories.
3.1.2. Quantum-geometry effects. We should then apply effective techniques to the Hamiltonian constraint of gravity, computing $\langle \hat{H}[N] \rangle$. Expressions for the Hamiltonian constraint are rather complicated even classically, given by
\[ H_{\text{grav}}(q_{ab}, \pi^{cd}) = -\frac{16\pi G}{\sqrt{\det q}} \left( \pi_{ab} \pi^{ab} - \frac{1}{2} (\pi_a^a)^2 \right) + \frac{\sqrt{\det q}}{16\pi G} (3) R \] (30)
in ADM variables, the spatial metric $q_{ab}$ and its momentum
\[ \pi^{cd} = \frac{\sqrt{\det q}}{16\pi G} (K^{cd} - K_q^{\kappa} q^{cd}) \]
in terms of extrinsic curvature (with the spatial Ricci scalar $(3) R$).

Loop quantum gravity uses a different set of variables, the densitized triad $E^a_i$ instead of the spatial metric $q^{ab} = E^a_i E^b_j / \det(q_{cd})$ and the Ashtekar–Barbero connection $A^a_i = \Gamma^a_i + \gamma K^a_i$ [43, 44], defined by combining the spin connection $\Gamma^a_i$ compatible with the densitized triad and extrinsic curvature $K^a_i = K_{ab} E^{bi}/\sqrt{|\det(E^j_i)|}$. The basic Poisson brackets are
\[ \{A^a_i(x), E^b_j(y)\} = 8\pi G \delta^a_b \delta^j_i \delta(x, y). \] (31)
The Barbero–Immirzi parameter $\gamma > 0$ [44, 45] does not play a role classically but appears in quantum spectra and corrections. In these variables, the Hamiltonian constraint is
\[ H_{\text{grav}}(A^a_i, E^b_j) = -\frac{E^a_i E^b_j \epsilon^{ij}_{k}}{16\pi G \det(E^j_i)} \left( F^k_{ab} + (1 + \gamma^{-2}) \epsilon^{k}_{mn}(A^m_n - \Gamma^m_n)(A^n_m - \Gamma^n_m) \right) \] (32)
with the curvature $F^k_{ab}$ of the Ashtekar–Barbero connection.

Both expressions are rather complicated to quantize, owing for instance to the expressions of $(3) R$ or $\Gamma^a_i$, to be written in terms of the metric or densitized-triad operators. Fortunately, there are several characteristic features, common to both versions: the Hamiltonian constraint is quadratic in the connection or extrinsic curvature, and it requires an inverse of the spatial metric or the densitized triad. These two features, when combined with quantum-representation properties, imply characteristic structures of quantum geometry and associated corrections to classical equations. These corrections, in turn, can be analyzed for potential implications even if their precise form cannot be determined from a complete calculation of $\langle \hat{H} \rangle$ in semiclassical states. And even if expectation values could be computed for a specific $\hat{H}$ and some states, ambiguities in the construction of $\hat{H}$ or the choice of states would be so severe that only general features and characteristic effects could be trusted.

In a Wheeler–DeWitt quantization, we have formal quantum constraint equations with $\pi_{ab}$ in (30) replaced by functional derivatives with respect to $q_{ab}$, acting on wave functions $\psi[q_{ab}]$. The formal nature leaves precise representation properties unclear, and therefore does not show specific quantum effects; one simply takes the classical expression and performs the usual substitution of momenta by derivative operators. One does not expect strong quantum-geometry effects, simply because quantum geometry has not been completed in this setting. Loop quantum gravity, on the other hand, has celebrated its greatest success so far at this level of quantum representations, and indeed sheds considerable light on questions of quantum corrections resulting from quantum geometry.

3.1.3. Loop representation and background independence. Loop quantum gravity looks closely at representation properties of basic operators. To eliminate the need for formal functional derivatives and the associated delta functions in quantizations of (31), the classical fields $A^a_i$ and $E^b_j$ are smeared or integrated over suitable sets in space: holonomies $h_t(A^a_i) = \mathcal{P} \exp(\int_0^t ds a^a_i A^a_i)$ and fluxes $F^{ij}_{ab}(E^b_j) = \int_S d^3y n^a_i E^b_j f^i$ with the tangent vector $t^i$ to a curve $e$ and the co-normal $n^a_i$ to a surface $S$ (on which an $su(2)$-valued smearing function
allowing for all curves and surfaces, all information about the fields can be recovered. By the integrations, the delta function in \( \{ \Lambda_i(x), E_j^f(y) \} = 8\pi \gamma G \delta^{ij} \delta(x, y) \) is eliminated, and a well-defined holonomy-flux algebra results:

\[
[h_\epsilon(A_i^f), F_j(E_j^f)] = 8\pi \gamma G h_{\epsilon\rightarrow\epsilon'}\tau_i f_i'(x)\tau_j
\]

if there is only one intersection point \( \{ x \} = e \cap S \), denoting by \( h_{\epsilon\rightarrow\epsilon'} \) and \( h_{\epsilon\rightarrow\epsilon''} \) the holonomy along \( e \) up to \( x \) and starting at \( x \), respectively. With strong uniqueness properties of possible quantum representations \([46–49]\), spatial quantum geometry in this setting is under excellent control.

Representations of the holonomy-flux algebra then provide operators to be inserted in (32) to obtain a quantized Hamiltonian constraint. The kinematical Hilbert space is spanned by cylindrical states \( \Psi(A_i^f) = \psi(h_{\epsilon}(A_i^f), \ldots, h_{\epsilon}(A_i^f)) \), each of which depends on the connection via a finite number of holonomies. The full state space, has no restriction on the number of holonomies that may appear, thereby representing the continuum theory rather than some lattice model. The inner product is obtained by integrating the product of two cylindrical functions over as many copies of \( SU(2) \) as there are non-trivial dependencies on holonomies in both states, using the normalized Haar measure. By completion of the space of cylindrical functions, the kinematical Hilbert space is obtained \([50]\). Holonomies \( h_\epsilon \) then act as multiplication operators, changing the dependence of a cylindrical state on \( h_\epsilon \), or creating a new dependence if the state was independent of \( h_\epsilon \) before acting. Flux operators, representing the densitized triad, become derivative operators in the connection representation used, and can be expressed in terms of invariant derivative operators on \( SU(2) \) (or angular-momentum operators). They have discrete spectra, indicating modifications to the classical spatial structure \([51–53]\): distance, areas or volumes computed from \( E_j^f \) can, after quantization, no longer increase continuously even if the underlying curves, surfaces, or regions are deformed by homotopies.

As a further consequence of discreteness, it turns out that holonomy operators do not continuously depend on the curves used. A cylindrical state depending only on \( h_\epsilon \) and one depending only on \( h_{\epsilon\rightarrow\epsilon'} \) with a piece \( \epsilon' \) appended to the curve refer to two different holonomies, and are orthogonal according to the inner product just described, even if \( \epsilon' \) is a one-point set. While we classically have \( t^\nu A_i^f(x)\tau_i = \lim_{\epsilon\rightarrow\epsilon'}(h_\epsilon(A_i^f) - 1)/|\epsilon'| \), where \( t^\nu \) is the tangent vector of \( \epsilon' \) at \( x \) and \( |\epsilon'| \) its coordinate length, the sequence \( h_\epsilon |\psi \rangle \) of states after quantization does not converge for any \( |\psi \rangle \) if \( \epsilon' \) is changed. The edge dependence disappears when one implements the diffeomorphism constraint, which has not been assumed in the previous constructions. States \( h_\epsilon |\psi \rangle \) for different \( \epsilon' \) are no longer orthogonal, but they all give rise to the same state when diffeomorphism is factored out. The limit can then be taken, but always equals zero. Again, there is no way of deriving a connection operator.

Unlike with classical expressions, it is not possible to take a derivative of \( h_\epsilon(A_i^f) \), for instance by the endpoint of \( \epsilon \), to obtain an expression for a quantized \( A_i^f \). Loop quantum gravity does not offer connection operators; all connection dependence in the Hamiltonian constraint must be expressed in terms of holonomies. No quadratic function as it appears in the constraint can exactly agree with a linear combination of exponentials, and modifications arise, motivated by background-independent quantum geometry.

### 3.1.4. Holonomy corrections.

When the Hamiltonian constraint is quantized in loop quantum gravity, holonomies are used instead of connection components \([35]\), providing a ‘regularization’ necessary to render the constraint expressible by basic operators. However, the limit in which the ‘regulator’—the specific curves used for holonomies—is removed does not exist; we are not dealing with a proper regularization. (In \([36]\), the limit is argued to exist and be trivial if spatially diffeomorphism-invariant states are used. But with this assumption
there is no handle on the full off-shell algebra and its anomaly problem.) Instead, one usually interprets the difference of a holonomy-modified constraint or its effective versions with the classical expression as a series of higher-order corrections, amending the classical Hamiltonian by higher powers of the connection, or intrinsic and extrinsic curvature. In this viewpoint, the modification is similar to expected higher-curvature corrections—except for the issue of covariance that we will have to address. (In some models of loop quantum cosmology, it is possible to represent an exponentiated version of the constraint in terms of holonomy operators without introducing modifications to the classical expression [54]. However, the procedure seems to depend sensitively on specific properties of the model used and is not available in general.)

Holonomy corrections therefore appear as higher-order terms such as

\[-2 \tau \text{Tr} (\tau_i h_c (A^i_j)) - \tau^a_i A^a_j (x) = -\frac{1}{24} (\tau^a_i A^a_j (x) (\tau^b_j A^b_i (x)) (\tau^c_j A^c_i (x)) + \tau^a_i \partial^b_j \partial^a_j A^a_j (x) + \cdots \]  

(34)

obtained from a Taylor expansion of the exponential and a derivative expansion of the integration. These terms depend on the routing of the curve \( e \), to be chosen suitably for a quantization of the Hamiltonian constraint. The condition of anomaly-freedom puts strong restrictions on the possible routings [55] which, however, are difficult to evaluate. Moreover, the expansion is done in an effective derivation, requiring the calculation of expectation values that lead to additional moment terms. All these calculations are difficult to perform explicitly, but the form of corrections is clear and quite characteristic: higher orders as well as higher spatial derivatives in the connection. With these types of corrections, suitably parameterized, one can look for consistent deformations of the constraint algebra to find versions for a physical evaluation of these corrections, or to derive further restrictions on the quantization choices made.

In effective equations, the use of holonomies as basic operators of the quantum theory has another consequence: the holonomy-flux algebra (33) is not canonical, with non-constant Poisson brackets. Moments of states used for effective descriptions are based on expectation values of basic operators, holonomies and fluxes in loop-quantized models. The general constructions of effective theories still go through: Poisson brackets on the quantum phase space, the quantum Hamiltonian or constraints, and so on. However, the explicit Poisson relations (24) evaluated between individual moments of the form \( \Delta (\hbar F^c) \) are different from the canonical case. In particular, moments no longer Poisson-commute with expectation values. This feature requires care and complicates some calculations. These problems, however, are only technical; see the examples provided later in section 4.3.2 and in [56, 57].

3.1.5. Inverse-triad corrections. Fluxes are linear in the densitized triad and do not suggest the same kind of modification as holonomies. Nevertheless, there is a characteristic effect associated also with them. Flux operators have discrete spectra, containing zero as an eigenvalue. Such operators do not have densely-defined inverses, and yet we need an inverse of the densitized triad for the classical Hamiltonian constraint. To obtain such quantizations, a more indirect route is taken in loop quantum gravity, which does result in well-defined operators but introduces another kind of correction, called inverse-triad correction.

To see the form of these corrections, we show a lattice calculation of inverse-triad operators. As proposed in [36, 58], the combination of triad components required for the Hamiltonian constraint (32) is first rewritten as

\[ 2\pi \gamma G e^{ijk} \epsilon_{abc} \frac{E^b_i E^c_k}{\sqrt{\det E}} = \left\{ A^i_k, \int \sqrt{|\det E|} \, d^3 x \right\}. \]  

(35)
In the new form, no inverse is needed, $A'_e$ can be expressed by holonomies, the volume operator can be used for $\int \sqrt{|\det E|} d^3x$, and the Poisson bracket be turned into a commutator divided by $i\hbar$. The resulting operators are rather contrived, especially with SU(2) holonomies and derivatives involved. But the presence of corrections and their qualitative form can be illustrated by a U(1)-calculation, for which we also assume regular cubic lattices.

On a cubic lattice, we can assign a unique plaquette to each link $e$, by which we then label fluxes. Our basic operators are $\hat{h}_e$, which as a multiplication operator by $\exp(i \int_A e^a d\lambda^a)$ takes values in U(1), and $\hat{F}_e$ for a fixed set of edges $e$ in a regular cubic lattice. We are therefore computing inverse-triad operators and their expectation values for a fixed subset of cylindrical states, but the lattice can be as fine as we want, allowing us to capture all continuum degrees of freedom. For this U(1)-simplification, the holonomy-flux algebra, quantizing an Abelian states, but the presence of corrections and their qualitative form can be illustrated by a U(1)-calculation, for which we also assume regular cubic lattices.

We first rewrite (35) in terms of holonomies instead of connection components, and express the volume $V = \int \sqrt{|\det E|} d^3x$ by lattice fluxes $\sqrt{|F_1 F_2 F_3|}$ per vertex, with the three fluxes through plaquettes in all three directions around the vertex: $e^a(V) = i\hbar, [h^{-1}, \sqrt{|F_1 F_2 F_3|}]$ or, more symmetrically, $i\hbar, [h^{-1}, \sqrt{|F_1 F_2 F_3|} - h^{-1} [h_e, \sqrt{|F_1 F_2 F_3|}]]$, computes the Poisson bracket at the vertex. Since $h_e$ commutes with all but one of the $F_i$, we can focus on one of them, $\sqrt{|F_i|}$. Keeping the power more general, the quantization of some inverse power of flux takes the form

$$\left(|F|^{-r-1} \text{sgn } F \right)_e = \frac{\hat{h}_e^r \hat{F}_e^r \hat{h}_e - \hat{h}_e \hat{F}_e^r \hat{h}_e^r}{16\pi G r \gamma \ell_p^2} =: \hat{I}_e.$$  \hfill (36)

For any $0 < r < 1$ we quantize an inverse power of $F$ but need not use any inverse in the commutator.

Following [59], we can now easily simplify these operators, if we observe the relations of the U(1)-holonomy-flux algebra, together with the reality condition. These relations imply

$$\hat{h}_e^r \hat{F}_e^r \hat{h}_e = |\hat{F}_e + 8\pi \gamma \ell_p^{-2}|^r, \quad \hat{h}_e \hat{F}_e^r \hat{h}_e = |\hat{F}_e - 8\pi \gamma \ell_p^{-2}|^r,$$

such that

$$\hat{I}_e = \frac{\hat{F}_e + 8\pi \gamma \ell_p^{-2}}{16\pi G r \gamma \ell_p^2} - \frac{\hat{F}_e - 8\pi \gamma \ell_p^{-2}}{16\pi G r \gamma \ell_p^2}.$$  \hfill (37)

Eigenvalues of this operator can easily be computed, with eigenstates equal to flux eigenstates [60, 61]. All eigenvalues are finite, as required for a densely-defined operator, and show how the classical divergence of $|F|^{-r-1}$ at $F = 0$ is cut off. For inverse-triad corrections in effective Hamiltonians, however, we need expectation values of $\hat{I}_e$ in semiclassical states. Explicit calculations would require good knowledge of semiclassical wave functions or coherent states.

For general effective equations it is sufficient, and even more useful, to perform a moment expansion, keeping the specific state free and parameterized by moments. Staying at the expectation-value order of effective expressions, we have

$$\langle \hat{I}_e \rangle = \frac{|\langle \hat{F}_e \rangle + 8\pi \gamma \ell_p^{-2} |^r - |\langle \hat{F}_e \rangle - 8\pi \gamma \ell_p^{-2} |^r}{16\pi G r \gamma \ell_p^2} + \text{ moment terms.}$$  \hfill (38)

Already to this order we see characteristic corrections (depending on $\hbar$ via the Planck length). Inverse-triad corrections therefore have a contribution independent of quantum back-reaction. Interpreting $\langle \hat{F}_e \rangle = \langle L \rangle$ as the discrete quantum-gravity scale (the lattice spacing as measured by flux operators), we find the correction function

$$a_r(L) := \frac{\langle \hat{I}_e \rangle - L^{2(r-1)}}{I_{\text{class}}} = \frac{L^2 + 8\pi \gamma \ell_p^{-2} |^r - L^2 - 8\pi \gamma \ell_p^{-2} |^r}{16\pi G r \gamma \ell_p^2} L^{2(1-r)}.$$  \hfill (39)
that will appear in an effective Hamiltonian constraint. To leading order in an expansion by \( \hbar \) (or \( \ell_P^2 L^2 \)), the correction function equals one. But even if no moment terms are included, there are quantum corrections in the full form of \( \alpha(L) \). Corrections are strong for \( L^2 \sim 8 \pi \gamma \ell_P^2 \) or smaller, typically in the deep quantum regime, where \( \alpha(L) \) drops to zero at \( L = 0 \). However, even for larger \( L \), \( \alpha_r(L) \) is not identical to one and implies interesting corrections.

In addition to corrections contained in (39) and quantum back-reaction from moment terms, the flux dependence implies corrections from a derivative expansion of the integrations involved, as already seen for holonomies. Moreover, non-Abelian holonomies do not lead to exact cancellations in the substitution of \( h e^{-1} e, V \) for \( t a e^{-1} e, V \) and rather imply additional higher-order corrections by powers of \( A_{ab} \) [62]. As noted in the context of holonomy corrections, such extra terms mix with higher-curvature corrections. The leading term in (39), on the other hand, shows a different dependence on parameters that distinguish a given cosmological regime and are more characteristic. Their effects can thus be studied in isolation.

### 3.2. Diffeomorphism constraint

We have already stated that the diffeomorphism constraint can be quantized by its direct action on spatial functions or other objects such as curves and surfaces. In loop quantum gravity, for instance, a diffeomorphism \( \Phi \) acts by shifting all arguments of a cylindrical function by \( h \rightarrow h \phi(\cdot) \), the usual pull-back of functions. The representation of the holonomy-flux algebra is diffeomorphism covariant under this action, showing that no quantum corrections to classical diffeomorphisms result. It is not possible to compute or represent an infinitesimal action or the diffeomorphism constraint because two states that differ by a non-trivial diffeomorphism are either identical (if the diffeomorphism does not change the underlying graph) or orthogonal. But finite diffeomorphisms suffice to remove the related gauge, which is done without quantum corrections.

Nevertheless, the situation is not completely satisfactory because the diffeomorphism constraint is a crucial ingredient of the hypersurface-deformation algebra. If diffeomorphisms are represented without quantum corrections, there should be no deformations of the relations (10) and (11) of the hypersurface-deformation algebra for commutators involving at least one spatial deformation. However, the diffeomorphism constraint also appears on the right-hand side of (12), the crucial part for space-time structure. On the left-hand side, we have two Hamiltonian constraints, which we do quantize in loop quantum gravity and whose commutators we can, in principle, compute. The result should be a well-defined operator, which must vanish on physical states for the quantization to be anomaly-free. However, classically it corresponds to a diffeomorphism constraint, which cannot be represented directly.

To check for anomaly freedom, one must then find an operator version of the right-hand side of (12), taking into account the structure function \( q_{ab} \), to be turned into an operator as well. This is one of the most important but still outstanding issues in loop quantum gravity, which was evaded by the arguments of [36] and only partially addressed by the advanced constructions of [63, 64]. More recently, the issue has been revisited in several models [55], with encouraging results. At least in \( U(1) \)-versions of 2 + 1-dimensional gravity, one can indeed make sense of the right-hand side of (12) as an operator, in such a way that the quantum constraint algebra is anomaly-free. As a side product, the same deformation (13) with inverse-triad corrections as seen by effective methods [11] appears. (Holonomy corrections and their deformation of the constraint algebra could not be seen by the methods of [55], going back to [63, 64], because the consistency conditions of anomaly freedom are tested only at vertices.)

In [55], the diffeomorphism constraint itself did not have to be amended by quantum corrections. However, other considerations in the same context have been put forward that...
may suggest such terms [65]. At present, the status regarding quantum corrections in the
diffeomorphism constraint is incomplete, but a consistent implementation does not appear
to be easy. From the point of view of effective theory, corrections to diffeomorphisms do
not seem required because, in any canonical space-time theory, one is dealing with fields as
functions on space. These functions are represented using some coordinates, but physics as
always must be independent of the choice. There must therefore be a part of the gauge content
of the theory that requires independence under arbitrary changes of spatial coordinates or,
infiniteresimally, invariance under spatial Lie derivatives. But then, a gauge transformation that
amounts to a Lie derivative of all fields must have a generator identical to the diffeomorphism
constraint uniquely associated with the fields [66]. The spatial structure assumed in canonical
formulations leaves no room for corrections in the diffeomorphism constraint.

The space-time structure is not presupposed in canonical quantum gravity and may well
change, as indicated by some quantum corrections in the Hamiltonian constraint. Space-time,
unlike space, has dynamical content and can easily receive quantum corrections, as borne out
in loop quantum gravity. Having the classical structure of space but modified space-time is
therefore consistent. Nevertheless, in an effort to relax some of the general assumptions of
canonical formulations, one could expect changes to the spatial manifold structure as well, as
perhaps indicated by potential corrections in the diffeomorphism constraint such as those in
[65].

3.3. Quantum-geometry effects

Comparing holonomy and inverse-triad corrections, we have several important properties.

- Holonomy corrections crucially add higher powers of the connection to the classical
  quadratic form of the Hamiltonian constraint. In flat isotropic cosmological models, the
  connection is proportional to the Hubble parameter $\mathcal{H}$, which in turn is proportional to
  the square root of the energy density. Holonomy corrections in cosmological models
  therefore depend on the dimensionless parameters $\ell_P \mathcal{H}$ or $\sqrt{\rho/\rho_P}$, both of which are tiny
  in observationally accessible regimes.

  Inverse-triad corrections, on the other hand, depend on the ratio $\ell_P^2 / L^2$ with the discrete
  quantum-gravity scale $L$ in (39). It is not easy to estimate $L$, but the dimensionless ratio
  associated with it certainly need not be small. Inverse-triad corrections can be more
  significant than holonomy corrections in observationally accessible regimes. (The scale $L$
  may change in time, depending on the form of lattice refinement realized [67, 68].)

- Holonomy corrections and inverse-triad corrections are both obtained from properties of
  integrated objects, holonomies and fluxes. One should therefore expect not just higher-
  order terms as in the expansions already discussed, but also higher spatial derivatives
  in a derivative expansion of inhomogeneous models. For holonomy corrections, higher-
  derivative terms are crucial because they should be part of higher-curvature corrections
  together with higher powers of the connection that immediately arise from expanded
  holonomies. Only a suitable combination of higher powers and derivatives can result in
  consistent covariant versions.

- Following up on the last item, we also need higher time derivatives to complete higher-order
  corrections to covariant objects related to curvature. Such corrections should be present
  even in homogeneous models, but are not easy to see directly from the form of holonomies.
  However, such terms cannot be ignored, because high-curvature regimes have significant
  contributions from higher-order and higher-derivative terms. In isotropic models, $\mathcal{H}^2$ and
  $\dot{\mathcal{H}}$ are of similar orders, both related to linear combinations of stress-energy components
  by the Friedmann and Raychaudhuri equations. An expansion of holonomies only by $\mathcal{H}$
(related to the isotropic connection; see section 4.2) but ignoring higher time derivatives would be inconsistent. To see how higher time derivatives arise in canonical quantum theories, we have to pause our description of loop quantum gravity and return to more details of quantum back-reaction.

4. Quantum back-reaction

For a canonical effective theory, quantum Hamiltonians and quantum constraints \( \langle \hat{H} \rangle \), generating evolution or gauge flows by (29), must be expanded systematically by moments of states to see all quantum effects. This is also the case for individual non-linear correction functions such as \( \langle \hat{I} \rangle \) of inverse triads (38) or \( \langle \hat{h} \rangle \) of holonomies as they may be implied by quantum-geometry effects of loop quantum gravity. Additional terms, products of expectation values and moments, are then added to the constraints.

4.1. Effective quantum mechanics

The correctness of the quantum dynamics resulting from a moment-expanded \( \langle \hat{H} \rangle \) can be illustrated with a quantum-mechanical example. We start with the well-known Ehrenfest equations

\[
\frac{d}{dt} \langle \hat{q} \rangle = \langle \hat{p} \rangle / m, \quad \frac{d}{dt} \langle \hat{p} \rangle = -\langle V' \rangle
\]

for basic expectation values, computed using (29). These equations have been analyzed by [69] in the limit \( \hbar \to 0 \) to prove that quantum mechanics has the correct classical limit. Effective equations go beyond this limit by performing a systematic expansion in \( \hbar \).

The first Ehrenfest equation takes exactly the classical form, while the momentum expectation value is subject to quantum corrections: \( \frac{d}{dt} \langle \hat{p} \rangle = -\langle V' \rangle \) does not equal the classical force \( F(\langle \hat{q} \rangle) = -V'(\langle \hat{q} \rangle) \) at position \( \langle \hat{q} \rangle \) (unless the potential is at most quadratic). Moments as quantifiers of corrections arise when we expand the quantum force \( F_Q = \frac{d}{dt} \langle \hat{p} \rangle \) as

\[
-\langle V' \rangle = -\frac{\partial V_Q}{\partial \langle \hat{q} \rangle}
\]

or the quantum potential as

\[
V_Q(\langle \hat{q} \rangle, \Delta(q^n)) = V(\langle \hat{q} \rangle + (\hat{q} - \langle \hat{q} \rangle)) = V(\langle \hat{q} \rangle) + \sum_{n=2}^{\infty} \frac{1}{n!} \frac{\partial^n V}{\partial \langle \hat{q} \rangle^n} \Delta(q^n)
\]

such that \( -\langle V' \rangle = -\partial V_Q / \partial \langle \hat{q} \rangle \).

4.1.1. Quantum Hamiltonian. The quantum potential is defined as a function on the infinite-dimensional quantum phase space of expectation values and moments, whose Poisson structure is given by (24). In a quantum Hamiltonian

\[
H_Q = \langle \hat{H} \rangle = \frac{1}{2m} (\langle \hat{p} \rangle^2 + \Delta(p^2)) + V_Q(\langle \hat{q} \rangle, \Delta(q^n)),
\]

we therefore have terms generating a dynamical flow of the moments by

\[
\Delta(q^n \hat{p}^r) = \{\Delta(q^n \hat{p}^r), H_Q\}.
\]
The coupled set of equations for expectation values and moments, (40) and (44), is equivalent to the Schrödinger flow of quantum mechanics, but its solutions do not provide wave functions but rather variables directly related to observations. It can be solved with different approximations, most importantly a semiclassical one by the order of moments, sometimes combined with an adiabatic one. In the latter case, applied to anharmonic oscillators, effective equations are equivalent to those of the low-energy effective action [30]. The validity and usefulness of the canonical effective scheme is thereby established.

In the context of quantum gravity, the feature of higher time derivatives in effective equations, a crucial ingredient of higher-curvature corrections, is of particular interest. The moments are related to such terms, although not in a direct way. Equation (40) combined with (41) already shows that a specific linear combination of the moments, with coefficients depending on expectation values, amounts to the time derivative of the momentum, or the second derivative of the position expectation value. Higher than second time derivatives of \( \langle \hat{q} \rangle \) can be computed by taking further derivatives of (40) and inserting \( \dot{\langle \hat{q} \rangle} \) and, for higher than third order, \( \dddot{\langle \hat{q} \rangle} \) according to equations of motion (44) generated by the quantum Hamiltonian. Different combinations of the moments therefore provide all higher time derivatives of \( \langle \hat{q} \rangle \).

With the scheme just sketched, it is difficult to invert the equations to find expressions for moments in terms of higher time derivatives, or to eliminate all moments and end up with a higher-derivative equation just for \( \langle \hat{q} \rangle \) instead of the moment-coupled (40), (41) and (44). But with more-refined methods, as well as an adiabatic expansion, this task can be performed. For quantum cosmology, we learn that we must study quantum back-reaction to see all terms relevant for higher-curvature corrections.

In semiclassical regimes, the moments by definition obey the \( \hbar \) hierarchy \( \Delta(q^k p^l) \sim O(\hbar^{(k+l)/2}) \), as can easily be verified in Gaussians; see (17) and [25]. We can therefore consider the first term \( \frac{1}{2}V''(\langle \hat{q} \rangle)(\Delta q)^2 \) for \( n = 1 \) in (42) as the leading semiclassical correction, providing a quantum Hamiltonian

\[
H_Q = (\hat{H}) = \frac{1}{2m}(\hat{p})^2 + V(\langle \hat{q} \rangle) + \frac{1}{2m}(\Delta p)^2 + \frac{1}{2}V''(\langle \hat{q} \rangle)(\Delta q)^2.
\]  

(45)

(The kinetic term contributes \( (\Delta p)^2/2m \), potentially of the same order as \( \frac{1}{2}V''(\langle \hat{q} \rangle)(\Delta q)^2 \). But it does not appear in a product with expectation values and therefore does not cause quantum back-reaction.) For equations of motion of expectation values and second-order moments, relevant to this order, we use the Poisson brackets (26). Applied to our second-order quantum Hamiltonian, we find

\[
\frac{d}{dt}(\langle \hat{q} \rangle) = \frac{\langle \hat{p} \rangle}{m}
\]

(46)

\[
\frac{d}{dt}(\langle \hat{p} \rangle) = - V'(\langle \hat{q} \rangle) - \frac{1}{2}V'''(\langle \hat{q} \rangle)(\Delta q)^2
\]

(47)

\[
\frac{d}{dt}(\Delta q)^2 = \frac{2}{m}\Delta(qp)
\]

(48)

\[
\frac{d}{dt}\Delta(qp) = \frac{1}{m}(\Delta p)^2 - V'''(\langle \hat{q} \rangle)(\Delta q)^2
\]

(49)

\[
\frac{d}{dt}(\Delta p)^2 = - 2V'''(\langle \hat{q} \rangle)\Delta(qp).
\]

(50)

For a given potential, one may solve these equations numerically. However, it would be more instructive to compute \( (\Delta q)^2 \) and insert it in (47) to see what quantum corrections result. So
far, all equations are coupled to one another and one cannot solve independently for \((\Delta q)^2\) (unless \(V''\) is constant, the case of the harmonic oscillator, a constant force or a free particle). But with an additional adiabatic approximation for the moments, decoupling can be achieved.

### 4.1.2. Adiabatic approximation

To zeroth order in an adiabatic approximation, we assume the moments (but not expectation values) to be time independent. We will denote the adiabatic order by an integer subscript. Equations (48) and (50) then imply \(\Delta_0(q_p) = 0\) at zeroth adiabatic order, and (49) shows that \((\Delta_0p)^2 = mV''(\langle \hat{q} \rangle)(\Delta_0q)^2\). With the last equation, we see that the zeroth-order adiabatic approximation cannot be valid unless \(\langle \hat{q} \rangle\) is constant in time as well. To avoid such a restrictive condition, we proceed to higher adiabatic orders, from order \(i\) to order \(i + 1\) by inserting time derivatives of \(\Delta_i(q^p_p)\) on the left-hand sides of (48)–(50) to compute \(\Delta_{i+1}(q^p_p)\) on the right-hand sides. (For a systematic implementation of the adiabatic approximation, see [30, 70].) With time derivatives known from preceding orders, the equations to solve for the moments are initially algebraic, but additional consistency conditions relating different orders sometimes imply differential equations for coefficients, as we will see in this example.

To first adiabatic order,

\[
\Delta_1(q_p) = \frac{1}{2} m \frac{d}{dt} (\Delta_0q)^2 = -\frac{1}{2V''(\langle \hat{q} \rangle)} \frac{d}{dt} (\Delta_0p)^2
\]

\[
= \frac{1}{2} \frac{V''(\langle \hat{q} \rangle)}{V''(\langle \hat{q} \rangle)} \frac{d}{dt} (\Delta_0q)^2 + \frac{d}{dt} (\Delta_0q)^2
\]

\[
= -\frac{1}{2} \frac{d}{dt} (\Delta_0q)^2
\]

using (48), (50) and our zeroth-order condition relating \((\Delta_0p)^2\) to \((\Delta_0q)^2\). The two lines can both hold only if

\[
\frac{d}{dt} (\Delta_0q)^2 = \frac{C}{\sqrt{V''(\langle \hat{q} \rangle)}}
\]

with a constant \(C\). Our zeroth-order adiabatic relation between the moments then shows that \((\Delta_0p)^2 = mV''(\langle \hat{q} \rangle)(\Delta_0q)^2 = mC\sqrt{V''(\langle \hat{q} \rangle)}\). Inserting these solutions in the quantum Hamiltonian (45), we obtain a correction

\[
\frac{1}{2m} (\Delta_0p)^2 + \frac{1}{2} \frac{V''(\langle \hat{q} \rangle)(\Delta_0q)^2}{\sqrt{V''(\langle \hat{q} \rangle)}} = C \sqrt{V''(\langle \hat{q} \rangle)}
\]

to the classical Hamiltonian.

As one goes to higher orders in the adiabatic approximation, one takes more and more time derivatives of \(\Delta_0(q^p_p)\). We can see this feature already with the low-order equations found here. So far, we have used the first adiabatic order only to restrict the zeroth-order solutions. But with the solution (54) found for \((\Delta_0q)^2\), we obtain from (51) the moment

\[
\Delta_1(q_p) = \frac{1}{2} \frac{d}{dt} (\Delta_0q)^2 = \frac{d}{dt} (\Delta_0q)^2 = \frac{1}{4} C \frac{V''(\langle \hat{q} \rangle)}{\sqrt{V''(\langle \hat{q} \rangle)}} \frac{d}{dt} (\Delta_0q)^2
\]

depending on a first-order derivative of \(\langle \hat{q} \rangle\). We do not need \(\Delta(q_p)\) in the quantum Hamiltonian, but this pattern continues for all moments at higher adiabatic orders, including \(\Delta_i(q^p_p)\). When we go beyond second adiabatic order and insert solutions into expectation-value equations, higher-derivative effective equations will be obtained; see [70] for explicit derivations. Quantum back-reaction by moments is responsible for these higher-derivative corrections.
but there is no direct correspondence between the moments as independent quantum degrees of freedom and new degrees of freedom that appear in higher-derivative equations because more initial values need to be specified. It is not the moment expansion itself which gives rise to higher derivatives, but rather the adiabatic expansion of individual moments. The order of moments corresponds to a semiclassical expansion, according to $\Delta(q^0 p^0) \sim O(h^{h/4)/2})$ in semiclassical states, not to a derivative expansion. Any fixed order in $\hbar$ can produce arbitrarily high orders of time derivatives if the adiabatic expansion is pushed further.

4.1.3. State dependence. The parameter $C$ in (54), related to second-order moments, is of the order $\hbar$ in semiclassical states; the correction (55) is therefore the first-order semiclassical correction under the assumption of zeroth adiabatic order for the moments. We cannot choose arbitrary values for $C$ because the uncertainty relation (18) must be obeyed, such that $C = m^{-1/2} \Delta_0 q \Delta_0 p \geq \frac{1}{2} \hbar / \sqrt{m}$. Requiring the uncertainty relation to be saturated determines $C$. In general, this condition may be too strong because we would assume saturation at all times, amounting to the existence of a dynamical coherent state which is not guaranteed for general potentials. But to zeroth adiabatic order, with the solutions found here, such an assumption is consistent: all dependence on $\langle \hat{q} \rangle$ drops out in the product of $(\Delta_0 q)^2 (\Delta_0 p)^2$ (and we have $\Delta_0 (q p) = 0$).

Without additional assumptions on the states solved for, or initial conditions for the moment equations (48)–(50), the constant $C$ remains undetermined. One possibility to fix $C$, in the class of models of this example, is to assume that solutions are close to the harmonic-oscillator vacuum or some other specific state. If the potential $V(q) = \frac{1}{2} m \omega^2 q^2$ is harmonic, $(\Delta_0 q)^2 = C / \sqrt{m} \omega^2$ is constant—in this case there are states for which the adiabatic approximation is exact—and equals the Gaussian spread $\sigma^2$ in a coherent state: we may write $C = \sigma^2 \sqrt{m} \omega^2$. For the harmonic oscillator, dynamical coherent states do exist and the uncertainty relation may be satisfied at all times. In this case, $C = \frac{1}{2} \hbar / \sqrt{m}$, or $(\Delta_0 q)^2 = \frac{1}{2} m \omega c$, the correct relation for position fluctuations in the ground state. With $(\Delta_0 p)^2 = \frac{1}{2} m \omega a$, the non-classical terms in the quantum Hamiltonian amount to the zero-point energy $\frac{1}{2} \hbar \omega$.

For a general potential $V$, we do not have the frequency parameter $\omega$ to refer to, but we can define it as the square root of $2/m$ times the coefficient of the quadratic term in a Taylor expansion $V(q) = V_0 + V_1 q + \frac{1}{2} m \omega^2 q^2 + \cdots$, assuming that the coefficient is not zero. In this way, we treat higher than second-order terms in the potential as an anharmonicity. Specifying the class of states solved for as those that are close to a harmonic-oscillator ground state, we can therefore write $(\Delta_0 q)^2 = \frac{1}{2} \hbar / \sqrt{m} V(q') / m$ in the effective Hamiltonian (55) then agrees with that found for the low-energy effective action [26], a relation that holds to higher adiabatic orders as well [30].

The canonical picture of quantum back-reaction provides an interpretation of moment-coupling terms as an analog of loop diagrams in quantum field theory, with moments taking the place of $n$-point functions. A formulation of the canonical effective scheme for quantum field theory is not fully worked out yet, but its implications for quantum gravity and cosmology can nevertheless be seen. Already in minisuperspace models there are characteristic effects which show cosmological implications of quantum corrections.

4.1.4. Notes on the WKB approximation. The WKB approximation is often seen as implementing a semiclassical regime, in the sense that leading terms in powers of $\hbar$ are considered in the quantum evolution equation for states, expanded as $\psi(q) =$
exp \((\hbar^{-1} \sum_{n=0}^{\infty} \hbar^n S_n(q))\) with an asymptotic series. With this ansatz in the Schrödinger equation, one can solve order by order in \(\hbar\) to find expressions for the \(S_n\): in quantum mechanics,

\[
\frac{1}{2m} \left(\frac{dS_0}{dq}\right)^2 + V(q) = E, \quad i \frac{dS_0}{dq} + \frac{2}{\hbar} \frac{dS_0}{dq} \frac{dS_1}{dq} = 0
\]

for zeroth and first order in \(\hbar\) implies \(S_1 = -\frac{1}{2} i \log(2m(E - V(q))) + \text{const}\), while \(S_0\) satisfies the classical Hamilton–Jacobi equation.

Solutions obtained by the WKB approximation do not directly provide observables such as expectation values, for which additional integrations would be necessary. Such integrations are usually complicated to perform not just analytically but also numerically, given the strongly oscillating nature of WKB solutions in semiclassical regimes. Moreover, WKB solutions do not show how quantum corrections can be included in classical equations as the dominant quantum effects. In particular, although quantum back-reaction is implicitly contained in solutions to the WKB equations, it does not appear in the form of effective potentials or quantum forces useful for intuitive explanations of quantum effects. In the WKB approximation, \(S_0\) satisfies exactly the classical Hamilton–Jacobi equation, without any quantum corrections. Corrections to the dynamics arise by higher orders of \(S_n\) in the wave function, but they do not appear in a form added to the Hamilton–Jacobi (or another classical) equation.

While the WKB approximation, as an expansion in \(\hbar\), does have a semiclassical flavor, it can more generally be viewed as a formal expansion to produce solutions for wave functions. The WKB equations are obtained by solving the Schrödinger equation exactly at every order of \(\hbar\): an equation \(\sum_{n=0}^{\infty} E_n \hbar^n = 0\) is interpreted as implying \(E_n = 0\) for all \(n\). From a semiclassical perspective, on the other hand, one would interpret an equation \(\sum_{n=0}^{\infty} E_n \hbar^n = 0\) as providing a tower of quantum corrections \(\sum_{n=0}^{\infty} E_n \hbar^n\) to the classical expression \(E_0\), and then be interested in solutions to the equations \(\sum_{n=0}^{N} E_n \hbar^n = 0\) cut off at finite orders of \(\hbar\). Additional consistency conditions are needed to determine the \(E_n\) showing up in quantum corrections. Usually, the \(E_n\) for \(n > 0\) depend on state parameters such as fluctuations, while \(E_0\) depends only on expectation values and equals the classical expression. A dynamical equation \(\sum_{n=0}^{\infty} E_n \hbar^n = 0\) then encodes the quantum back-reaction of state parameters on the expectation values, implying deviations from classical behavior, as derived systematically by effective equations.

In principle, one could derive such quantum corrections from WKB solutions by computing expectation values of the \(\hbar\)-expanded wave functions. But the WKB approximation does not automatically arrange the terms in its equation by semiclassical relevance. While canonical effective equations have a direct correspondence to the low-energy effective action, as already seen, the WKB approximation does not produce all terms [71]. Another question, important in the context of quantum gravity and quantum cosmology, is the treatment of quantum constraints (or the physical Hilbert space), which remains open in the context of WKB solutions. (For instance, one may solve \(\hat{H}\psi = 0\) with WKB techniques, but for approximate solutions, the gauge flow \(\exp(-i\hat{H}[\epsilon]/\hbar)\psi_{\text{WKB}}\) does not automatically vanish.) Canonical effective techniques, on the other hand, apply to constrained systems as well and even help to solve some long-standing conceptual problems of quantum gravity related to constraints and gauge.

4.1.5. Effective constraints and the problem of time. As already indicated in section 3.1.1, a quantum constrained system with constraint operators \(\hat{C}\) produces quantum constraints \(C_Q := \langle \hat{C}\rangle\), defined just like a quantum Hamiltonian (43), but also independent quantum phase-space functions \(C_f = \langle (f(\hat{q}, \hat{p}) - (f(\hat{q}, \hat{p}))\hat{C}\rangle\) (in this ordering) constrained to vanish in physical states [37, 38]. In semiclassical expansions, calculating order by order in the
moments, polynomial \( f(q, p) \) are sufficient. To fixed order in the moments, only finitely many constraints are then present. Their number is larger than the number of classical constraints because they remove not only expectation values of constrained degrees of freedom but also the corresponding moments.

With the ordering of constraint operators to the right of \( f(q, p) \) chosen in effective constraints, they are automatically first class if the constraint operators are first class. There are then constraint equations to be solved, and gauge flows to be factored out. The gauge flow is computed using the Poisson brackets (24), affecting also the moments. Standard techniques of constrained systems can then be used, except that moments truncated to a fixed order is computed using the Poisson brackets (24), affecting also the moments. Standard techniques are then constraint equations to be solved, and gauge flows to be factored out. The gauge flow constraints, they are automatically first class if the constraint operators are first class. There the corresponding moments.

To see the treatment of effective constraints we consider a Hamiltonian constraint operator \( \hat{C} = \hat{p}^2 - \hat{p}^2 + W(\phi) \) for a free, massless relativistic particle \((q, p)\) coupled to a second degree of freedom \((\phi, p_\phi)\) with an arbitrary \(\phi\)-dependent potential \(W(\phi)\). Depending on the form of \(W(\phi)\), \(p_\phi\) may become zero along trajectories generated by the Hamiltonian constraint, in which case \(\phi\) does not serve as global internal time. On the other hand, with a \(q\)-independent Hamiltonian constraint, we could deparameterize by \(q\), obtaining evolution by the classical Hamiltonian \(p = \pm \sqrt{p_\phi^2 + W(\phi)}\). We have equations of motion \(d\phi/dq = \pm p_\phi/\sqrt{p_\phi^2 + W(\phi)}\) and \(dp_\phi/dq = \mp \frac{1}{2} W(\phi)/\sqrt{p_\phi^2 + W(\phi)}\). The momentum \(p_\phi\) evolves, and could indeed become zero.

The constraint operator gives rise to the effective constraints \([40, 41]\)

\[
C_Q = \langle \hat{p}_\phi \rangle^2 - \langle \hat{p} \rangle^2 + (\Delta p_\phi)^2 - (\Delta p)^2 + W((\hat{\phi})) + \frac{1}{2} W''((\hat{\phi}))(\Delta \phi)^2
\]  

(58)

\[
C_\phi = 2\langle \hat{\phi}\rangle \Delta (p_\phi) + i \hbar \langle \hat{p}_\phi \rangle - 2 p \Delta (\phi p) - W((\hat{\phi}))(\Delta \phi)^2
\]  

(59)

\[
C_{p_\phi} = 2\langle \hat{\phi}\rangle (\Delta p_\phi)^2 - 2\langle \hat{p}\rangle \Delta (p_\phi p) + W'((\hat{\phi}))(\Delta (p_\phi)) - \frac{1}{2} i \hbar
\]  

(60)

expanded to second order in the moments, together with additional constraints \(C_q, C_p, C_{qp}\) and so on, which we will not make use of. These constraints can be solved to find the quantum-corrected constraint surface, and their gauge flows can be computed to find moments of observables in physical states. Once the non-symplectic nature of the Poisson manifold of second-order moments is taken into account, these calculations are not very different from standard procedures.

The effective constraints shown here illustrate another important feature: the complexity of constraints and their solutions. It comes about because effective constraints, to be first class, are defined in a non-symmetric ordering, while moments are by definition Weyl ordered. Reorderings required to express effective constraints as functions of the moments then introduce imaginary contributions by the commutator \([\hat{q}, \hat{p}] = i \hbar\). For \(C_\phi \) and \(C_{p_\phi} \), to vanish, some moments must be complex. While moments before the imposition of constraints, belonging to a kinematical Hilbert space, should be real as the expectation values of Weyl-ordered operators, after solving the constraints one moves to the physical Hilbert space, in general not related to a subspace of the kinematical one. After solving the constraints, the original kinematical moments may therefore take complex values, as long as physical observables of the quantum constrained system are subject to reality conditions.

For further consequences, we study the problem of time in this system, using the variable \(\phi\) as internal time even though it does not deparameterize the system globally. At the full quantum level, local internal times, free of turning points only for finite ranges of evolution,
cannot easily be made sense of: if internal time exists only for a finite range, evolution cannot be unitary even in this range. (See for instance the discussion in [72–74].) If states are evolved by local internal times past their turning points, evolution freezes: expectation values are stuck at constant values [75, 76].) This consequence is the reason why the problem of time is much more severe at the quantum level, compared to the classical one. At the effective level, as we will see, the problem of time can be overcome, allowing consistent derivations of observables without using artificial deparameterizations [40–42].

If \( \phi \) is used as (local) internal time, it is not represented as an operator on the resulting physical Hilbert space, whatever it may be. No generally manageable techniques are known to derive physical Hilbert spaces and evolution in non-deparameterizable systems (for some possibilities of Hilbert-space derivations, see e.g. [75–78]). At the effective level, it is sufficient to distinguish \( \phi \) as non-operator time by requiring that its moments in effective constraints vanish,

\[
(\Delta \phi)^2 = \Delta (\phi q) = \Delta (\phi p) = 0
\]  

while its expectation value \( \langle \phi \rangle \) (denoted without the hat to indicate that \( \hat{\phi} \) no longer acts as an operator) will become the time parameter. In fact, the conditions (61) implement a good gauge fixing of the second-order constraints \( C_\phi, C_p, C_q \) and \( C_p \) after quantization. (With constraints on a non-symplectic Poisson manifold, only three gauge-fixing conditions are required for four constraints. The remaining second-order moment involving \( \phi, \Delta (\phi p_\phi) \), is fixed by the constraints, as we will see shortly.) In the terminology of [40], these conditions implement the Zeitgeist during which \( \phi \) as local internal time is current. Imposing (61) initiates the transition to physical moments—moments computed for states in the physical Hilbert space on which \( \phi \) does not act as an operator.

Solving the effective constraints in the given Zeitgeist, we have \( \Delta (\phi p_\phi) = -\frac{1}{2}i\hbar \) from \( C_\phi = 0 \), which then implies

\[
(\Delta p_\phi)^2 = \frac{\langle \hat{p} \rangle^2}{\langle \hat{p}_\phi \rangle^2}(\Delta p)^2 + \frac{1}{2} \frac{W'(\langle \phi \rangle)\hbar}{\langle \hat{p}_\phi \rangle}
\]

from \( C_p = 0 \). Inserted in (58), this implies the reduced constraint

\[
C = \langle \hat{p}_\phi \rangle^2 - \langle \hat{p} \rangle^2 + \frac{\langle \hat{p} \rangle^2 - \langle \hat{p}_\phi \rangle^2}{\langle \hat{p}_\phi \rangle^2}(\Delta p)^2 + \frac{1}{2} \frac{W'(\langle \phi \rangle)\hbar}{\langle \hat{p}_\phi \rangle} + W(\langle \phi \rangle)
\]  

amounting to the quantum constraint \( C_Q = \langle \hat{C} \rangle \) on the space on which \( C_\phi \) and \( C_p \) are solved in the given Zeitgeist. Solving \( C = 0 \) for \( \langle \hat{p}_\phi \rangle \), we obtain the time-dependent Hamiltonian for \( \langle \phi \rangle \)-evolution, including quantum back-reaction. However, it still contains complex terms.

In (62), all terms except the last two are expected to be real-valued because \( \langle \hat{p} \rangle \) and \( \Delta p \) are physical observables, and \( \langle \hat{p}_\phi \rangle \) can be interpreted physically as the local energy value. The constraint can then be satisfied, only if we allow for an imaginary part of \( \langle \phi \rangle \), calculated from

\[
\frac{1}{2} \frac{W'(\langle \phi \rangle)\hbar}{\langle \hat{p}_\phi \rangle} + W(\langle \phi \rangle) = 0.
\]

For semiclassical states, to which this approximation of effective constraints refers, we can Taylor expand the potential

\[
W(\langle \phi \rangle) = W(\text{Re}(\phi) + i\text{Im}(\phi)) = W(\text{Re}(\langle \phi \rangle) + i\text{Im}(\langle \phi \rangle)W'(\text{Re}(\langle \phi \rangle)) + O((\text{Im}(\langle \phi \rangle))^2)
\]

by the imaginary term, expected to be at least of the order \( \hbar \) because it vanishes classically. To this order, the imaginary contribution \( \text{Im}C = 0 \) to \( C \) in (62) implies that

\[
\text{Im} \langle \phi \rangle = -\frac{\hbar}{2\langle \hat{p}_\phi \rangle}.
\]
The remaining terms,
\[
\text{Re } C = \langle \hat{p}_\phi \rangle^2 - \langle \hat{p} \rangle^2 + \langle \hat{p}_\phi \rangle^2 + \langle \hat{p}_\phi \rangle^2 (\Delta p)^2 + W(\text{Re } \langle \phi \rangle) = 0 \quad (65)
\]
provide the physical \( \text{Re } \langle \phi \rangle \)-Hamiltonian upon solving the constraint equation for \( \langle \hat{p}_\phi \rangle \). At this stage, the Hamiltonian and its solutions, corresponding to evolving observables with respect to \( \phi \), are all real: physical reality conditions are imposed and we have solutions corresponding to states in the physical Hilbert space.

Although imaginary parts may be unexpected, a detailed analysis of this and other models shows that they are fully consistent [41]. In models in which one can compute a physical Hilbert space, results equivalent with those shown here are obtained. Within the effective treatment of constraints, if we transform to a different internal time such as \( q \), which is done by a gauge transformation in the effective constrained system so that a new Zeitgeist—the gauge-fixing (61)—is realized, the imaginary parts are automatically transferred from \( \langle \phi \rangle \) to \( \langle q \rangle \), in such a way that observables remain real. By successive gauge transformations, one can evolve through turning points of local internal times, without freezing the evolution of physical observables; see in particular the cosmological example analyzed in [42]. The imaginary part of time can be seen as a remnant of non-unitarity problems of evolution in local-time quantum systems, but unlike in Hilbert-space treatments, it does not pose any problems at the effective level.

Gauge transformations in effective constrained systems show that physical results are independent of the choice of (local) internal time. One may deparameterize the effective system in different ways to solve the resulting equations, without affecting observables. This conclusion, one example for effective solutions to the traditional problems of canonical quantum gravity, indicates that deparameterization can be used consistently. However, in complicated systems subject to ambiguities such as factor-ordering choices, each deparameterization must be formulated in a specific way so that they all can result from one non-deparameterized system, effective or not. At the effective level, all quantum constraints and Zeitgeists must be computed and implemented with the same operator \( \hat{C} \) for different local time choices to produce mutually consistent results. In many constructions of physical Hilbert spaces, however, one quantizes a system with a specific deparameterization in mind, choosing factor orderings and using possible simplifications. In such a case, there is no guarantee that results can agree with those obtained from other parameterizations, and the independence of physical results of the choice of time is put at risk.

4.2. Modified Friedmann equations, or: the sins of sines

In quantum cosmology, a systematic derivation of quantum back-reaction is required especially for reliable evaluations of holonomy corrections in the Hamiltonian constraint, as they both are relevant in high-curvature regimes and contribute to higher-curvature terms. Constraints appear in such systems, but for simplicity we will refer to deparameterized toy models. Holonomy corrections have provided a popular class of models within loop quantum cosmology, in which the Friedmann equation is modified in a simple way [79]: the classical constraint equivalent to the Friedmann equation is first modified to
\[
H_{\text{mod}} = -\frac{3}{8\pi G} \frac{\sin^2(\ell\epsilon)}{\gamma^2\ell^2} \sqrt{|\rho| + p|p|^{3/2}} = 0 \quad (66)
\]
with a holonomy parameter \( \ell \) that could possibly depend on \( p \). According to loop quantum cosmology [80, 4], the Hamiltonian is written in canonical triad and connection variables, with \( A'_i = c\delta^\phi_i \) and \( E^a_i = p\delta^\phi_i \), \( \{c, p\} = 8\pi \gamma G / 3 \), under the assumption of isotropy. The densitized-triad component \( p \) can be positive and negative, according to the orientation of
the triad, and is related to the scale factor by \(|p| = a^2\). (Without loss of generality regarding effective equations, we take \(p\) to be positive in what follows.) For spatially flat models, as assumed here, \(c = \gamma \dot{a}\) is proportional to the proper-time derivative of the scale factor. By the modification in (66), the periodic form of holonomies is implemented, replacing the quadratic connection dependence of the classical expression.

Computing Hamiltonian equations of motion for \(p\) allows us to eliminate \(c\) in favor of \(\dot{p}\), upon which the constraint equation takes the form of some kind of Friedmann equation. We have \(p = \{p, H_{\text{mod}}\} = (\gamma \ell c)^{-1} \sin(2\ell c) \sqrt{\rho}\). Using trigonometric identities, we find \(\sin^2(\ell c) = \frac{1}{2}(1 - \sqrt{1 - 4\gamma^2 \ell^2 c^2})\) with \(\dot{a} = \dot{p}/(2\sqrt{\rho})\). Inserting this in the modified constraint and solving for \(\dot{a}^2\), the modified Friedmann equation becomes

\[
\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3} \rho \left(1 - \frac{8\pi G}{3} \gamma^2 \ell^2 a^2 \rho\right). \tag{67}
\]

This simple and interesting equation, with just a quadratic correction to the energy density, has served as the basis of many ad hoc investigations of potential effects of loop quantum cosmology.

Equation (67) is clearly not an effective equation in the generality written here. Quantum back-reaction is ignored, while all terms in the complete series expansion of holonomy corrections

\[
\frac{\sin^2(\ell c)}{(\ell c)^2} - 1 = -\frac{1}{3} \ell^2 c^2 + \frac{4}{45} \ell^4 c^4 + \ldots \tag{68}
\]

are taken into account for the calculation. A consistent treatment would include only those higher-order terms in an expansion of holonomy modifications that are larger than any quantum back-reaction or other term that has been ignored. The relation of quantum back-reaction to higher-curvature corrections indicates that \(c^2\)-corrections in (68) should be of comparable size to \(\dot{c}\)-corrections from quantum back-reaction, the latter of which are not included in (67).

Including holonomy corrections but ignoring quantum back-reaction is therefore inconsistent, even at leading order in the \(c\)-expansion, unless one considers only models in which quantum back-reaction is weak. (Such models do indeed exist, as we will show later, but they are very special.) Keeping all terms in the \(c\)-expansion to arbitrary orders then leads to a questionable equation.

One could think that keeping small higher-order terms is harmless, but it turns out that our cautionary considerations do matter for the form of modified Friedmann equations. To see this concretely, let us look at a few examples in which the holonomy modification in the Hamiltonian constraint is expanded first, followed by a calculation of Hamiltonian equations of motion and a modified Friedmann equation. The first order of \(c\)-corrections provides a constraint

\[
H_1 = -\frac{3}{8\pi G} \frac{c^4}{\gamma^2} \left(1 - \frac{1}{3} \ell^2 c^2\right) \sqrt{\rho} + \rho \dot{c}^{3/2} = 0. \tag{69}
\]

Proceeding as before, we compute \(\dot{p} = \{p, H_1\} = 2\gamma^{-1}c(1 - \frac{2}{3} \ell^2 c^2) \sqrt{\rho}\), solve for \(c\) in terms of \(\dot{p}\), insert the result in \(H_1\), and rewrite as

\[
\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3} \rho \left(1 - \frac{8\pi G}{3} \gamma^2 \ell^2 a^2 \rho\right). \tag{70}
\]

Rather surprisingly, the result agrees exactly with the one obtained with the full holonomy modification, (67). However, this outcome does not mean that higher orders in the \(c\)-expansion do not matter. It rather shows that the specific form of the full modification by \(\sin^2(\ell c)\) is arranged so delicately that all higher-order contributions beyond the \(c^2\)-correction precisely
cancel one another. To confirm this, we go one order beyond the quadratic correction, modifying
the Hamiltonian constraint by
\[ H_2 = -\frac{3}{8} \frac{c^2}{\gamma^2} \left( 1 - \frac{1}{3} \ell^2 a^2 + \frac{4}{45} \ell^4 a^4 \right) \sqrt{\rho} + \rho \frac{\dot{\rho}}{\rho}^{3/2} = 0. \] (71)

Again we proceed as before. (The higher higher-order polynomial equations to be solved for
a relation of \( c \) to \( \dot{\rho} \) can be handled easily within the perturbative scheme of the \( c \)-expansion.)
The result,
\[ \left( \frac{\ddot{a}}{a} \right)^2 = \frac{8\pi G}{3} \rho \left( 1 - \frac{8\pi G}{3} \gamma^2 \ell^2 a^2 \rho + \frac{157}{45} \left( \frac{8\pi G}{3} \right)^2 \gamma^4 \ell^4 a^4 \rho^2 \right). \] (72)

now has a higher-than-quadratic correction in the energy density. Going to higher orders in \( c \)
and following this scheme shows that also the energy-order increases to include all possible
powers. The leading corrections in \( \rho \), such as \((8\pi G/3)\gamma^2 \ell^2 a^2 \rho\) with the same coefficient
in all modified Friedmann equations, do not change if one goes to higher orders in the
\( c \)-expansion and can therefore be used consistently—provided one stays in energy ranges in
which it is the dominant term. When the energy density approaches Planckian levels and
holonomy corrections are strong, however, \( 8\pi G \gamma^2 \ell^2 a^2 \rho \) is close to one and all terms in the
energy expansion are relevant. Bounce scenarios, for instance, cannot be formulated with a
consistent version of the equation. (In this context, notice that the next term beyond \( \rho^2 \) enters
with a positive sign. At high density, it may well be larger than the correction in (67), in which
case no zero of \( \dot{a} \) and no bounce would be reached.)

As anticipated, the sine-modification has its infinitely many higher-order terms arranged
such that all but the quadratic energy correction disappear. A consistent perturbative treatment
keeping only the relevant orders instead produces a whole series expansion by the energy
density. If one has reasons to trust the whole sine function and to exclude all other corrections,
(67) is correct. But if there are additional corrections, however weak, it is not consistent to keep
all terms in a \( c \)-expansion of the sine function; instead, one has a modified Friedmann equation
with a perturbative expansion in \( \rho \). Those additional corrections then unbalance the fine balance
in the sine terms that eliminated all \( \rho \)-corrections beyond second order, and their form must be
known for a reliable derivation of correct effective Friedmann equations. The main source of
such extra terms is, of course, quantum back-reaction, producing higher time derivatives that
compete with higher powers of \( c \). (Higher orders are also sensitive to quantization ambiguities,
as analyzed for instance in [81].)

4.3. Harmonic cosmology

To understand the interrelation between different corrections, we should have a more detailed
look at quantum back-reaction in quantum cosmology. In an effective description of Wheeler–
DeWitt minisuperspace models, one considers the dynamics of expectation values \( \langle \dot{a}\rangle \) and
\( \langle \dot{p}_\phi \rangle \) coupled to fluctuations and higher moments \( \Delta (a^m \dot{p}_\phi) \). The coupled dynamics, including
quantum back-reaction, is usually complicated and unruly, but it simplifies considerably if
perturbations around a simple model such as the harmonic oscillator in quantum mechanics
can be used. As an analog of the harmonic oscillator in quantum mechanics with simple
effective equations, quantum cosmology has a harmonic model given by a free, massless
scalar in a spatially flat isotropic geometry [56].

To realize the model as one with a Hamiltonian generating evolution, we must pick a
time variable which we do by parameterizing, using the scalar \( \phi \) as time. Since it is free and
massless, the Hamiltonian constraint
\[ H(a, p_a, p_\phi) = -\frac{2\pi G}{3} \frac{p_\phi}{a} + \frac{1}{2} \frac{\dot{\phi}^2}{a^2} \] (73)
implies that $p_\phi$ is a constant of motion and $\phi$ has no turning points where $p_\phi$ would move through zero. The scalar therefore provides a global internal time. Deparameterized models, as discussed before, cannot produce reliable physical predictions unless one can show that results do not depend on the choice of time. In the present context, we use the model merely to illustrate properties of quantum cosmological dynamics. For realistic effects, one can avoid deparameterization before quantization and the dependence on time choices by using effective constraints instead of effective deparameterized Hamiltonians [37, 38, 40, 41].

It is an interesting coincidence that the same model is easily deparameterizable and at the same time, as we will see, harmonic, without quantum back-reaction. Both features imply that the model is extremely special even among symmetry-reduced isotropic systems; its implications must therefore be interpreted with a great amount of care.

We perform deparameterization by solving the Hamiltonian constraint $H(a, p_a, p_\phi) = 0$ for

$$p_\phi(a, p_a) = \pm \sqrt{\frac{4\pi G}{3}} |ap_a|,$$

(74)

the Hamiltonian generating evolution with respect to $\phi$. Equations of motion for $a(\phi)$ and $p_a(\phi)$ are then obtained via Poisson brackets with $p_\phi(a, p_a)$. If solutions are to be transferred back to coordinate time, such as proper time, we solve $dp/\mathrm{d}x = \{\phi, H(a, p_a, p_\phi)\} = p_\phi/a(\phi)^3$ for $\phi(\tau)$ (with a constant $p_\phi$) and insert this function in our solutions for $a(\phi)$ and $p_a(\phi)$.

4.3.1. Effective Wheeler–DeWitt equations. Effective deparameterized equations are generated by the quantum Hamiltonian $\langle p_\phi(\hat{a}, \hat{p}_a)\rangle$,

$$\frac{d}{d\phi} \langle \hat{O} \rangle = \langle i\hbar \{\hat{O}, p_\phi(\hat{a}, \hat{p}_a)\} \rangle = \langle i\hbar \{\hat{O}, p_\phi(\hat{a}, \hat{p}_a)\} \rangle$$

(75)

using the Poisson brackets (24). The absolute value in $p_\phi(a, p_a)$ makes a completely general expansion in moments complicated, but for $|p_\phi|$ not close to zero, there is a simple effective Hamiltonian. If we can ensure positivity of $\hat{a} \hat{p}_a$ in evolved states, the absolute value can be dropped. This is possible in particular for an initial state supported solely on the positive part of the spectrum of $\hat{a} \hat{p}_a$ (an operator for which we will assume Weyl ordering). Since $ap_a$ is preserved by the motion it generates, also after quantization, the evolved state will remain supported on the positive part of the spectrum of $\hat{a} \hat{p}_a$. Unless $|p_\phi|$ is close to zero, it is easy to find initial states supported only on the positive part of the spectrum of $\hat{a} \hat{p}_a$ and with specified initial expectation values for $\hat{a}$ and $\hat{p}_a$: projecting out negative contributions will not change the basic expectation values much. We are then allowed to write (75) as

$$\frac{d}{d\phi} \langle \hat{O} \rangle = \pm \sqrt{\frac{4\pi G}{3}} \langle \{i\hbar \hat{O}, \hat{a} \hat{p}_a\} \rangle = \pm \sqrt{\frac{4\pi G}{3}} \langle \{i\hbar \hat{O}, \hat{a} \hat{p}_a\} \rangle$$

(76)

using $|\hat{a} \hat{p}_a\rangle_+ = \hat{a} \hat{p}_a |\psi\rangle_+$ (and $|\hat{a} \hat{p}_a\rangle_+ = \hat{a} \hat{p}_a^{-1} |\psi\rangle_+$) on states $|\psi\rangle_+$ with support only on the positive part of the spectrum of $\hat{a} \hat{p}_a$.

On such positively supported states, the $\phi$-Hamiltonian is quadratic and can easily be expanded in moments. We have the quantum Hamiltonian

$$H_Q = \pm \sqrt{\frac{4\pi G}{3}} (\langle \hat{a} \rangle \langle \hat{p}_a \rangle + \Delta(a p_a)),$$

(77)
free of coupling terms of expectation values and moments: there is no quantum back-reaction. We compute and solve equations of motion for expectation values, resulting in

\begin{equation}
\langle \hat{a} \rangle (\phi) = \exp(\pm \sqrt{\frac{4\pi}{3}G} \phi) \quad \text{and} \quad \langle \hat{p}_a \rangle (\phi) = \exp(\mp \sqrt{\frac{4\pi}{3}G} \phi).
\end{equation}

To transform to proper time, we solve \( d\phi/d\tau = p_\phi \exp(\mp \sqrt{12\pi G}\phi) \) for

\begin{equation}
\phi(\tau) = \pm \log(\pm \sqrt{\frac{12\pi}{G}p_\phi \tau}) \sqrt{12\pi G}
\end{equation}

and obtain \( \langle \hat{a} \rangle (\tau) = (\pm \sqrt{12\pi Gp_\phi \tau})^{1/3} \), the classical dependence on proper time with a stiff matter source. (In particular, even after Wheeler–DeWitt quantization the system remains singular: infinite density \( p_\phi^3/(2\langle \hat{a} \rangle^3) \) is reached at finite proper time.)

In addition to these expectation-value solutions, the state evolves such that its second-order moments change by

\begin{equation}
\frac{d}{d\phi} (\Delta a)^2 = \pm 2 \sqrt{\frac{4\pi G}{3}} (\Delta a)^2, \quad \frac{d}{d\phi} (\Delta p_a)^2 = \mp 2 \sqrt{\frac{4\pi G}{3}} (\Delta p_a)^2
\end{equation}

and \( d\Delta(a p_a)/d\phi = 0 \), with solutions such that \( (\Delta a)/\langle \hat{a} \rangle \) and \( (\Delta p_a)/\langle \hat{p}_a \rangle \) are constant. Semiclassicality is preserved exactly throughout evolution in this harmonic model, even at high density. Note that \( \Delta a \) and \( \Delta p_a \) change nonetheless, but have often been assumed constant when state evolution was modeled by Gaussians. Wrong quantum corrections then result, which is especially significant in the presence of quantum back-reaction when the harmonic model is generalized. Especially curvature fluctuations are important because they grow when one evolves to high density, and they do show up in effective constraints such as (20) as a simple example. This issue is another illustration of the importance of complete effective equations including the moment dynamics.

With additional ingredients such as spatial curvature, a cosmological constant, a scalar mass or self-interaction, anisotropy or inhomogeneity, the system is no longer harmonic and becomes subject to quantum back-reaction. Deviations from the classical trajectory will then occur, to be captured by effective equations. (Some of these ingredients also remove deparameterizability, but at the effective level we can still use local internal times.)

With a cosmological constant, for instance, the \( \phi \)-Hamiltonian becomes \( p_\phi(a, p_a) = \pm \sqrt{\frac{4\pi G}{3}} a \sqrt{p_a^2 - 4\Delta a^2} \), a non-quadratic expression that entails coupling terms between expectation values and moments in a quantum Hamiltonian.

### 4.3.2. Harmonic loop quantum cosmology

At first sight, it seems that quantum-geometry corrections in loop quantum cosmology imply quantum back-reaction by deviations from the quadratic nature if (66) is used. This expectation is correct for inverse-triad corrections, but holonomy corrections, although they change the quadratic nature by higher-order terms, still lead to a harmonic model free of quantum back-reaction [56].

To see this, we first change to connection variables \( c = \gamma \hat{a} = -(4\pi \gamma G/3)p_\gamma/a \) and \( p = a^2 \), with \( \{c, p\} = 8\pi \gamma G/3 \). The \( \phi \)-Hamiltonian is still quadratic in these variables, proportional to \( |c|p \), but the holonomy modification leads us to replace \( c \) by \( \sin(\ell c)/\ell \) with some \( \ell \) that may depend on \( p \). After this, the Hamiltonian \( p_\phi(c, p) \) is no longer quadratic in \( c \) and \( p \). However, if we introduce a new variable \( J := 3p \exp(i\ell c)/8\pi \gamma G \), we have a linear \( \phi \)-Hamiltonian

\begin{equation}
p_\phi = \pm 2 \sqrt{\frac{4\pi G}{3}} \frac{|\text{Im} J|}{\ell}
\end{equation}
Moreover, and importantly, we have a (non-canonical) closed algebra of basic variables, so that the \( \phi \)-Hamiltonian remains linear (and is just multiplied with \( 1 - x \) compared to (81)).

Moreover, and importantly, we have a (non-canonical) closed algebra of basic variables,

\[
\{V, J\} = -i\ell_0 J, \quad [V, \hat{J}] = i\ell_0 \hat{J}, \quad [J, \hat{J}] = 2i\ell_0 V, \tag{83}
\]

with the Hamiltonian a linear combination of the generators.

Given these properties, upon quantization the Ehrenfest equations still provide closed equations for expectation values, without coupling to moments and quantum back-reaction. The Hamiltonian operator

\[
\hat{p}_\phi = \pm \sqrt{\frac{4\pi G}{3}} (1 - x) \left( \frac{\hat{J} - \hat{J}^\dagger}{i\ell_0} \right) \tag{84}
\]

is linear in \( \hat{J} \) and its adjoint, and the quantum Hamiltonian is linear in \( \hat{J} \) and its complex conjugate. The only additional condition to impose is a reality condition because we have used partially complex variables. If we initially keep \( J \) and \( \hat{J} \) as independent variables, valid solutions must satisfy \( JJ - V^2 \).

We quantize by turning \( V \) and \( J \) into operators, choosing an ordering of \( J \) with the exponential to the right. The classical Poisson algebra is then replaced by the closed commutator algebra

\[
[V, \hat{J}] = \ell_0 h \hat{J}, \quad [V, \hat{J}] = -\ell_0 h \hat{J}, \quad [\hat{J}, \hat{J}] = -\ell_0 h (2\hat{V} + \ell_0 h), \tag{85}
\]

where the last \( h \) comes from reordering exponentials. (Note that this non-canonical algebra implies \( (V, J) \)-moments not commuting with expectation values on the quantum phase space.) The reality condition, with the same ordering, reads \( \hat{J}\hat{J} - V^2 = 0 \), which implies conditions on moments upon taking an expectation value, possibly preceded by multiplication with basic operators. For second-order moments, we have

\[
|\langle \hat{J} \rangle|^2 - (\langle \hat{V} \rangle + \ell_0 h/2)^2 = \Delta V^2 - \Delta \langle J \hat{J} \rangle + \frac{1}{4}\ell_0^2 h^2. \tag{86}
\]

(For conditions on higher moments, see [82].) The reality condition is a Casimir of the commutator algebra of type sl(2, \( \mathbb{R} \)) and therefore commutes with the quantum Hamiltonian proportional to \( i(\hat{J} - \hat{J}^\dagger) \). If reality holds for initial expectation values and moments, it holds at all times. This statement is true not only for the harmonic model but for any Hamiltonian because the Casimir commutes with all \( \hat{V}, \hat{J}, \) and \( \hat{J}^\dagger \) individually, and therefore with any function of these variables.

Solutions for expectation values obtained from the linear quantum Hamiltonian are

\[
\langle \hat{V} \rangle (\phi) = A \exp(C\phi) + B \exp(-C\phi) \quad \text{and} \tag{87}
\]

\[
\langle \hat{J} \rangle (\phi) = A \exp(C\phi) - B \exp(-C\phi) + \frac{i\ell_0}{C} p_\phi, \tag{88}
\]

with two integration constants \( A \) and \( B \) as well as the constant \( C = \pm 2\sqrt{3\pi G/\ell} (1 - x) \). The reality condition then requires that

\[
|\langle \hat{J} \rangle|^2 - \langle \hat{V} \rangle^2 = -4AB + \frac{\ell_0^2 p_\phi^2}{C^2}. \tag{89}
\]
is of the order $\langle \hat{V} \rangle \ell_0 \phi$ (the size of semiclassical fluctuations $\Delta V^2$ and $\Delta (J \dot{J})$ in (86)), much smaller than $p_\phi^2$ for a universe which has a large amount of matter and is semiclassical at least once. (Recall that it is sufficient to impose the reality condition at just one time, for instance when semiclassicality is realized.) The product $A B$ must therefore be positive, close to $\ell_0^2 p_\phi^2 / C^2$, and the function $\langle \hat{V} \rangle (\phi) \propto \cosh(C \phi - C \phi_0)$ never becomes zero. Holonomy modifications in the harmonic model replace the classical singularity by a bounce.

As already seen in the beginning of this section, the bounce property of holonomy-modified constraints, one can put effective equations into the form of quantum Friedmann equations. In the case of modifications in the harmonic model, in which moments enter just by the reality condition, not by quantum back-reaction. The quantum Friedmann equation is valid in this form only if the sole matter source is a free, massless scalar, and there is no spatial curvature, a cosmological constant, or deviations from isotropy. When any one of these conditions is violated, quantum back-reaction results and there is no spatial curvature, a cosmological constant, or deviations from isotropy. When any one of these conditions is violated, quantum back-reaction results and

\[ \dot{a} / a = \frac{8 \pi G}{3} \rho_{\text{free}} \left( 1 - \frac{8 \pi G}{3} \gamma^2 (\ell a)^2 \rho_0 \right). \]  

(92)

Except for the fluctuation terms in $\rho_0$, this is equation (67).

There is another, more important difference: the derivation of (92) holds only in the harmonic model, in which moments enter just by the reality condition, not by quantum back-reaction. The quantum Friedmann equation is valid in this form only if the sole matter source is a free, massless scalar, and there is no spatial curvature, a cosmological constant, or deviations from isotropy. When any one of these conditions is violated, quantum back-reaction results and

\[ \left( \frac{\dot{a}}{a} \right)^2 = \frac{8 \pi G}{3} \left( \rho - \frac{8 \pi G}{3} \gamma^2 (\ell a)^2 \rho_0 \right) \pm \frac{1}{2} \sqrt{1 - \frac{8 \pi G}{3} \gamma^2 (\ell a)^2 \rho_0 \eta W + \frac{d^2 W^2}{2 p_\phi^2} \eta^2} \]  

(93)
where $W(\phi)$ is a possible scalar potential, and we have a general quantum parameter $\eta = \sum_k \eta_k (a^k W/p_\phi^2)^k$ with coefficients $\eta_k$ that depend on the moments, especially correlation parameters [83, 84]. The expansion by $a^6 W/p_\phi^2$ can be interpreted as one by $(\rho - P)/(\rho + P)$ with pressure $P$. (For a free, massless scalar, $\rho = P$.) A more-specific evaluation requires the detailed computation of quantum back-reaction to analyze how the moments evolve and what values they take especially at high density. Techniques for numerical studies have been provided in [82].

While it is difficult to find general information about the values of moments, it is clear that they contribute, among other effects, the canonical analog of higher-time derivatives as they appear in higher-curvature corrections. Moment terms and quantum back-reaction should therefore be large in high-density regimes, near the big bang. Reliable results in loop quantum cosmology can only state that the singularity is avoided by a bounce when matter is kinetic dominated, in which case $W \ll \rho_{\text{kin}}$ and the $\eta$-dependent terms in (93) can be ignored unless $\eta$ is extremely large. This conclusion coincides with numerical investigations [85–87] of the underlying difference equation for wave functions. However, such numerical studies suffer from the choices required for wave functions, for instance by an initial state. With such methods, it is difficult to capture general-enough effects, which in quantum cosmology with its lack of distinguished states make robust conclusions difficult. As shown by the generality of the quantum Friedmann equations displayed here, effective techniques allow one to draw conclusions and confirm the regime-dependent validity of some effects even when no specific states are chosen.

4.3.4. Cosmic forgetfulness and signature change. There are additional and more-surprising properties of the high-density regime that invalidate a traditional bounce interpretation even in the harmonic model. First, staying in the isotropic context, there is cosmic forgetfulness [88, 89]: when crossing the bounce in $\phi$-evolution, some moments change in ways so sensitive to initial values that the pre-bounce state cannot be recovered precisely from what may be known post bounce. Using solutions of moment equations [89] or considerations of semiclassical wave functions [90], one can derive an inequality

$$
\left|1 - \frac{(\Delta V)_{\phi \to \infty}}{(\Delta V)_{\phi \to -\infty}}\right| \leq \frac{\Delta p_\phi/(\hat{p}_\phi)}{(\Delta V/(V))_{\phi \to \infty}}
$$

bounding the ratio of volume fluctuations at early and late times. For a state with fluctuations symmetric around the high-density regime near the minimum of $(V(\phi))$, the left-hand side would be near zero. The estimate can therefore be used to shed light on the question of how much a quantum state may change while evolving through high density, and how much possible changes can be controlled.

With matter fluctuations $\Delta p_\phi/(\hat{p}_\phi)$ usually much larger than geometry fluctuations $(\Delta V/(V))_{\phi \to \infty}$ at large volume, where quantum field theory on curved space-time should be a good approximation, the right-hand side of the inequality is much larger than one, and $(\Delta V)_{\phi \to \infty}$ can differ significantly from $(\Delta V)_{\phi \to -\infty}$. The inequality can be saturated by highly squeezed dynamical coherent states [89], showing that control on pre-bounce fluctuations cannot be improved unless states are restricted further, more strongly than by semiclassicality.

Several classes of specific states, especially ones with weak correlations of the canonical variables—the volume and the Hubble parameter—show more-symmetric behavior of volume fluctuations. Most wave functions that can be constructed explicitly, for instance using sl(2, $\mathbb{R}$)-coherent states based on the algebra (85) as used in [91], are only weakly correlated and do not show all possible asymmetries. Again, the effective viewpoint using moments instead of wave functions provides larger generality. And even though wave functions are not provided...
in explicit terms, one can show that wave functions for the moment solutions even at saturation of (94) do indeed exist: examples for such states are dynamical coherent states [57] saturating the uncertainty relation, whose existence can be shown by general methods well-known from quantum mechanics.

The second feature preventing a bounce interpretation brings us back to quantum space-time structure. For a reliable cosmological model, we must embed a holonomy-modified isotropic version within a consistent deformation of the constraint algebra. Only then can we be sure that the model describes consistent evolution of quantum space-time. No complete extension of holonomy corrections to inhomogeneity is known, but as we will see in the next section, existing versions of holonomy modifications at high density imply drastic modifications with signature change, turning space-time into a quantum version of four-dimensional Euclidean space. This happens right where the bounce would be, but without time and evolution in Euclidean space, a bounce interpretation is not valid even though the model remains non-singular.

5. Quantum geometry and dynamics of space-time

So far, in section 3, we have seen the quantum geometry of space, with its characteristic features of discrete structures in loop quantum gravity. To fit these modifications into a covariant quantum space-time structure, we must find a consistent deformation of the hypersurface-deformation algebra of which the modified Hamiltonian constraint is a part. As has by now become clear from many examples, derived at different levels of effective and operator calculations, the classical constraint algebra is then indeed deformed: quantum-geometry corrections imply modified quantum space-time structures [11]. The possibility of such deformations has also been suggested based on Wheeler–DeWitt quantization [92]. Instead of the classical commutator of two time deformations, we have

$$\{H[N_1], H[N_2]\} = D[\beta q^{ab}(N_1 \nabla b N_2 - N_2 \nabla b N_1)]$$

(95)

with a phase-space function $\beta \neq 1$.

The typical and rather universal form of these deformations is as follows. Holonomy corrections result in a curvature-dependent $\beta(K) = \cos(2\ell K)$, where $\ell$, related to the quantum-gravity scale $L$, is a holonomy parameter depending on the curves used to integrate the connection, and $K$ is a curvature component such as the Hubble parameter for perturbations around isotropic models [93] or the rate of change of orbit areas in spherical symmetry [94, 95]. Such a deformation has also been found by operator calculations in 2 + 1-models [96]. For inverse-triad corrections, $\beta = \alpha^2$ depends on the inverse-triad correction function $\alpha$ as in (39), which in turn depends on the quantum-gravity scale $L$ [11, 94, 95]. Also here, operator calculations have provided supporting evidence [55].

5.1. Example: spherical symmetry

Spherically symmetric models with their reduced number of free fields provide an interesting testing ground for different quantum space-time structures, and at the same time allow physical applications for instance to black-hole physics. In Ashtekar–Barbero variables, used to compute deformations with corrections from loop quantum gravity, we express the canonical structure by four fields, two scalars $A_\phi$ and $E^x$ and two densitized scalars $A_\lambda$ and $E^\phi$. They appear as components of spherically symmetric SU(2)-connections

$$A = A_\lambda(x)\tau_3 \text{dx} + A_\phi(x) \tilde{A}_\lambda \text{d} \theta + A_\phi(x) A_\lambda \sin \theta \text{d} \varphi + \tau_3 \cos \theta \text{d} \varphi$$

(96)
and densitized triads

\[ E = E^i(x)\tau_3 \sin \theta \frac{\partial}{\partial x} + E^\varphi(x)\tilde{\Lambda}^E \sin \theta \frac{\partial}{\partial \varphi} + E^\psi(x)\Lambda^E \frac{\partial}{\partial \psi}. \] (97)

For the general derivation see [97, 98, 4].

The \( \text{su}(2) \)-valued fields \( \Lambda^E = \tau_1 \cos(\xi(x)) + \tau_2 \sin(\xi(x)) \) and \( \tilde{\Lambda} = \tau_1^{-1} \Lambda \tau_3 \) describe a U(1)-gauge freedom with gauge rotations by \( \exp(\lambda(x)\tau_3) \), remnant from the initial SU(2)-freedom. Similarly, the densitized triad has independent \( \text{su}(2) \)-matrices \( \Lambda^E \) and \( \tilde{\Lambda}^E \). Also \( A_3 \) is affected by these gauge transformations, under which it changes to \( A_3 + d\xi/\lambda \) like a U(1)-connection, but the combination \( A_3 + d\xi/G \) is invariant, and happens to agree with an extrinsic-curvature component \( K_x \) (up to a factor of \( \gamma \)).

With different matrices \( \Lambda^E \) and \( \tilde{\Lambda}^E \), the components \( E^\varphi \) and \( A_3 \), unlike \( E^i \) and \( A_4 \), are not canonically conjugate. However, if we switch to extrinsic curvature also for \( \varphi \)-components, we obtain canonical pairs \( \{K_x(x_1), E^i(x_1)\} = 2\gamma G\delta(x_1, x_2) \) and \( \{K_\varphi(x_1), E^\varphi(x_2)\} = \gamma G\delta(x_1, x_2) \), as shown in [99]. In these canonical variables, we have the diffeomorphism constraint

\[ D_{\text{grav}}[N^i] = \int dx N^i (2K'_\varphi E^\varphi - K_x E^i) \] (98)

and the Hamiltonian constraint

\[ H[N] = - \frac{1}{2G} \int dx N[E^i]^{-1/2}(1 - \Gamma^2_x + K^2_\varphi)E^\psi + 2|E^i|K_\psi K_x + 2|E^i|\Gamma^2_\varphi, \] (99)

with \( \Gamma_\varphi = -(E^i)/2E^\psi \) a spin-connection component. (Primes denote derivatives by \( x \).)

The appearance of inverses of \( E^i \) and quadratic expressions in \( K_x \) and \( K_\psi \), the latter as canonical and gauge-invariant versions of the connection, suggests inverse-triad and holonomy corrections from loop quantum gravity. Hamiltonian constraint operators have been constructed in [99], and more generally for Gowdy models in [100, 101], in which inverse-triad operators and holonomy operators indeed appear. An effective Hamiltonian would be obtained from expectation values of these operators, but the calculations are complicated. Moreover, so far these Hamiltonians could not be ensured to be anomaly-free at the operator level. Instead, we can parameterize effective Hamiltonians by correction functions originating from inverse-triad and holonomy operators, and compute Poisson brackets of the modified constraints to see under which conditions they can be anomaly-free [94].

We write a general modified Hamiltonian constraint as

\[ H^Q_{\text{grav}}[N] = - \frac{1}{2G} \int dx N(\alpha|E^i|^{-1/2}E^\psi f_1(K_\psi, K_x) + 2\bar{\alpha}|E^i|^{1/2} f_2(K_\psi, K_x)) \]
\[ + \alpha^2|E^i|^{-1/2}(1 - \Gamma^2_x)E^\psi + 2\bar{\alpha}^2\Gamma^2_\psi|E^i|^{1/2}. \] (100)

with inverse-triad correction functions \( \alpha, \bar{\alpha}, \alpha^T \) and \( \bar{\alpha}^T \) initially left independent of one another, and holonomy correction functions \( f_1 \) and \( f_2 \). All these functions may in principle depend on all canonical variables, although the triad dependence of inverse-triad correction functions and the curvature dependence of holonomy correction functions should be primary. Moreover, an anomaly-free commutator with the diffeomorphism constraint shows that inverse-triad correction functions can only depend on \( E^i \), not on the density-weighted \( E^\psi \).

Computing Poisson brackets of two modified Hamiltonian constraints with different lapse functions, it turns out that anomaly freedom can be realized if \( f_1 = F^2_1 \) and \( f_2 = K_x F_2 \) provided that \( F_2 = F_1(\partial F_1/\partial K_\psi)\alpha/\bar{\alpha}^T \) [94]. Choosing a function \( F_1 \) periodic in \( K_\psi \), holonomy modifications for this component are realized. The second correction function \( F_2 \) is then fixed, showing how anomaly-freedom can put restrictions on possible modifications and quantum corrections. In fact, the corrections seem even stronger for the \( K_x \)-dependence, left unmodified
in the function \( f_2 \) shown here. An extension to a holonomy-corrected \( K \)-dependence appears more difficult than one of the \( K \)-dependence. Moreover, while \( K \) would give rise only to pointwise exponentials \( \exp(i\gamma tK_x) \) as holonomies, the curve integration along angular directions, in which \( K \) points, being trivial in spherically symmetric models, \( K \) would be replaced by a holonomy \( \exp(i\gamma \int dxK_x) \) integrated along some interval \( I \). Derivative corrections should therefore result as well, or the constraint would become non-local if integrations are left unexpanded.

If we take \( F_1(K_x) = \gamma^t \sin(\gamma tK_x) \), suitable for holonomy corrections as in the cosmological example (66), we have \( F_2(K_x, E^i) = (2\gamma t)^{-1} \sin(2\gamma tK_x)\alpha/\alpha^i \). The algebraic deformation is then given by \( \beta(E^i, K_x) = \bar{\alpha}\bar{\alpha}\partial F_2/\partial K_x \ [94] \). For the example provided, this means \( \beta(E^i, K_x) = \alpha(E^i)\alpha(E^i/\alpha^i(E^i)) \cos(2\gamma tK_x) \), a function that is negative for \( \gamma tK_x \sim \pi/2 \), at curvatures where the correction function \( f_1 \) is near its maximum and a strong modification of the classical linear function. This property is realized generically: combining the previous equations, we can write

\[
\beta(E^i, K_x) = \frac{1}{2} \bar{\alpha}\bar{\alpha} \frac{\partial^2 f_1}{\partial K_x^2}
\]

which is negative around maxima of \( f_1 \), irrespective of its functional form. Consequences of negative \( \beta \) will be discussed in more detail soon. Note also that holonomy corrections and inverse-triad corrections are rather independent of each other in their effect on the deformation, affecting \( \beta \) multiplicatively.

The inverse-triad correction functions must satisfy

\[
(\bar{\alpha}\bar{\alpha} - \alpha\bar{\alpha}^i)(E^i) + 2(\bar{\alpha}\bar{\alpha}^i - \bar{\alpha}\bar{\alpha}^i)E^i = 0
\]  

for a closed constraint algebra [94]. If \( F_1 \) is independent of \( E^i \), or at least depends on this triad variable in a way different from inverse-triad corrections, one can show that both terms in (102) must vanish individually, and we have \( \alpha_i = \alpha \) and \( \bar{\alpha}_i = \bar{\alpha} \). See also [102].

For consistent deformations in the presence of cosmological perturbations, anomaly-freedom is implemented in the same spirit, but with an extra ingredient. Without any symmetry assumptions, requiring irregular lattices and non-Abelian SU(2)-features, it is complicated to derive inverse-triad operators or to parameterize holonomy corrections. One therefore starts using all information about such correction functions that can be obtained in tractable models, such as a homogeneous background, and inserts those background functions just like \( \alpha \), \( \bar{\alpha} \), \( \alpha^i \), \( \bar{\alpha}^i \), \( f_1 \) and \( f_2 \) in spherically symmetric models. These functions refer only to the background variables, but depending on the order of cosmological perturbations, also the dependence on inhomogeneity is required. The corresponding terms, in many cases, cannot be computed directly from operators; instead, one inserts 'counterterms' in the Hamiltonian constraint expanded by inhomogeneity, taking into account all possible terms to the given order that could be generated by correction functions depending on homogeneous fields [11]. Terms that cannot be computed from operators are left unspecified as free functions. In many cases, counterterms contribute derivative corrections, adding for instance terms containing \( \partial E^i/\partial \partial K_x \) for inverse-triad corrections. A dependence of correction functions on integrated variables such as fluxes is therefore realized even if \( \alpha \) initially depends only on local triad values. The condition of anomaly-freedom is often so restrictive that the counterterms can be derived uniquely from known inverse-triad or holonomy correction functions of the background. Consistent constraints can therefore be computed even if not all quantum corrections are known in detail.

Another small difference between spherical symmetry and cosmological perturbations is the treatment of the SU(2)-gauge. In spherical symmetry, (98) and (100) are manifestly invariant under these transformations, even after deformation by quantum corrections. In perturbative treatments, on the other hand, one usually fixes a background triad, including
its SU(2)-gauge. But then, one can see that physical results and the deformation of the space-time algebra are independent of the specific SU(2)-fixing chosen. The constructions are therefore consistent even if some gauge has been fixed: All gauge fixings produce the same results. (The same arguments can be applied to the time gauge used to descend from space-time tetrads to spatial triads.) Such consistent derivations in the presence of gauge fixing are possible in simple cases such as the Gauss constraint, which moreover survives unmodified after quantization. Making gauge-fixings consistent is much less trivial if attempted for complicated constraints such as $H[N]$. First, it is difficult to find any good gauge fixing in general terms; having to study even all possible gauge fixings and to make sure that physical results do not depend on the choice is then nearly impossible. In such cases, the only manageable approach is to forgo gauge fixing before quantization or deformation, even if it makes derivations more complicated than in one given gauge.

5.2. The meaning of deformed hypersurface deformations

The hypersurface-deformation algebra encodes the space-time structure of generally covariant theories just as the Poincaré algebra encodes special relativity’s structure. One can recover the Poincaré relations by using functions $N$ and $N^a$ linear in some coordinates amounting to Minkowski space-time or a local Minkowski patch. For instance, two linear lapse functions of the form $N = \Delta t + \vec{v} \cdot \Delta \vec{x}$, inserted in (12), provide the commutator of Lorentz boosts by velocity $v$ and time translations $\Delta t$. Inserting two such functions, $N_1 = \vec{v} \cdot \Delta \vec{x}$ and $N_2 = \Delta t - \vec{v} \cdot \Delta \vec{x}$, on the right-hand side of (12) shows a commutator that amounts to the displacement $\Delta \vec{x} = \vec{v} \Delta t$.

In terms of linear hypersurface deformations, the relation follows from elementary geometry; see figure 1.

If the algebra is deformed, as in (13), the same choice of linear deformations along the normals gives rise to a rescaled relation $\Delta x = \beta v \Delta t$. Quantum space-time, with its discrete structure that is responsible for the algebraic deformation via holonomy and inverse-triad corrections, changes the relation between velocity and displacement; discrete space-time speeds up or slows down motion. Such a phenomenon is well-known from condensed-matter physics and should not come as a surprise, although the form in which it is realized here is rather different owing to the more-basic notions of space and time involved.

When $\beta$ becomes negative, as happens with holonomy corrections at high density, the relation $\Delta x = \beta v \Delta t$ is rendered counter-intuitive. However, the change of sign can be interpreted easily if one redraws figure 1 in Euclidean space, especially regarding the directions
of normals to spatial slices. As shown in figure 2 compared with figure 1, the displacement then indeed points in the opposite direction (and does not change magnitude). The relation \( \Delta x = -\nu \Delta t \) does not describe motion but rather, despite the notation of variables, a rotation. When \( \beta \) turns negative, we have Euclidean signature rather than Lorentzian. Even if \( \beta \) is not exactly \(-1\) but negative, the structure is best described as Euclidean even though we do not have classical Euclidean space (just as we do not have classical Minkowski space if \( \beta \) is positive but not exactly \(+1\)).

Signature change is not only a drastic reminder that we cannot take much of our usual concepts for granted when space-time is quantized. It also shows the limitations of approaches in which gauge-fixing or deparameterization is used before quantization or modifications of the constraint. If one fixes the gauge before quantization, one can only assume the classical space-time structure, which does not allow signature change. After gauge fixing and quantization, the full space-time structure can no longer be accessed, leaving one with the conclusion that space-time is unmodified. However, since the constraints are modified in quantization after gauge fixing and determine the gauge and space-time structure, the procedure becomes intrinsically inconsistent. Deparameterization cannot capture all quantum space-time effects either. When one distinguishes a phase-space degree of freedom to measure change and evolution, there is no guarantee that this degree of freedom actually behaves like time in a space-time sense. Also Euclidean theories can formally be deparameterized (internal time simply parameterizes gauge orbits of the Hamiltonian constraint), showing that deparameterized ‘evolution’ does not necessarily imply evolution in a temporal sense. Again, only a complete analysis of the off-shell constraint algebra, without eliminating some of its more complicated ingredients by gauge-fixing or deparameterization, can show what space-time structure is realized.

In our diagrams so far, we have assumed that normals are drawn using either Minkowski or Euclidean geometry. We did not use quantum corrections of angles even though distances and displacements did receive corrections as a consequence of the algebra (13). One may expect angles to change too, in particular angles of normals to spatial slices drawn to visualize the commutator of two time deformations. Such corrections could indeed happen, in general deformations of space-time structures, but since the angle between space and time directions would be involved, they would amount to deformations of the commutator (11) of a time and a space deformation. A temporal and a spatial deformation commute up to a temporal deformation, as illustrated in figure 3. If there are quantum corrections to this relation, one might interpret them as modified spatial displacements, rescaled compared to the classical relations, or a modification in space-time angles used to define temporal deformations along
the normals. In the former case, also the purely spatial commutator (10) should be modified, which is not the case. A modified (11) therefore indicates quantum corrections to space-time angles, not just to distances as indicated by a modified (12). For instance, modifications which add a term of $D[\beta NN']$ to the classical result of $[H[N], D[N^a]]$, as possible for vector modes [103] but not with scalar modes [93], would have an additional spatial shift of the open circles in (3). (Note that figure 3 also illustrates the fact that (11) is not subject to a change in sign in Euclidean signature. If the normals are drawn according to Euclidean geometry, just the rescaling of $\Delta x$ under boosts changes, but not the direction of the temporal displacement.)

Based on algebraic calculations in effective loop quantum gravity, modifications of (11) that seemed possible for vector modes subject to holonomy corrections [103] turned out not to be consistent with scalar modes [93]. It therefore appears that space-time angles are not affected by the corrections of loop quantum gravity, but as discussed in section 3.2, stronger corrections to the diffeomorphism constraint than used so far may be realized. For now, all consistent deformations point to quantum corrections only in the commutator of two time deformations.

5.3. Consistency and space-time structures

With a deformed hypersurface-deformation algebra the theory is fully consistent. The full amount of gauge transformations exists to remove spurious degrees of freedom, and constraints are guaranteed to be preserved by evolution. Cosmological observables, for instance, can be computed by standard Hamiltonian means, as developed for deformed algebras in [11, 104]. (The classical Hamiltonian formalism for cosmological perturbations, of [105], assumed certain features of observables that are modified by deformations.)

However, other familiar notions used often in general relativity no longer apply. Even the line element, one of the most basic mathematical objects of differential geometry, must be treated with care—or altogether avoided. Constraints obeying a modified algebra generate gauge transformations for metric components $q_{ab}$ that cannot agree with Lie derivatives or space-time coordinate transformations—otherwise, the form of gauge transformations would imply the classical hypersurface-deformation algebra. But if $q_{ab}$, or the space-time metric $g_{\mu\nu}$ completed in the usual way using lapse and shift in

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu = -N^2 dt^2 + q_{ab}(dx^a + N^a dt)(dx^b + N^b dt), \quad (103)$$

does not transform by classical coordinate changes, the contraction $g_{\mu\nu} dx^\mu dx^\nu$ with standard coordinate differentials $dx^\mu$ is not invariant and cannot be used as a line element. One would have to modify transformations of coordinate differentials as well to make the contraction
invariant, in which way one could possibly make contact with non-commutative [106] or fractional geometry [107]. (Modified hypersurface-deformation algebras have also been found with higher-derivative dispersion relations for matter [108], but the form does not appear related to what is suggested by loop quantum gravity.)

Lacking a line element and related notions such as geodesics or trapped surfaces, black-hole properties and even their definitions must be rethought. One can only rely on canonical formulations of horizon conditions that capture the well-known notions of standard space-time. Classically, there are several different definitions of horizons which, at least in simple cases, all provide the same results. However, when they are reformulated canonically and adapted to quantum space-time, results may differ. As analyzed in [109], the consistency of quantum space-time structures also in this case helps to arrive at unambiguous answers.

For calculations in quantum space-time, one must rely on Hamiltonian methods, using directly the modified constraints. First applied systematically in [104], one obtains unambiguous expressions for gauge-invariant variables in cosmology as well as their evolution equations. Without using an action, it may not always be obvious how to combine all equations obtained to just one Mukhanov-type equation for the analog of the curvature perturbation, but examples have been found for inverse-triad corrections [110] and holonomy corrections [111]. Quantum corrected wave equations are then obtained, which directly show the modified speeds of modes as expected from a deformed hypersurface-deformation algebra: electromagnetic and gravitational waves obey the equation

\[- \frac{\partial^2 w}{\partial t^2} + \beta \Delta w + f(a, \dot{a})w = 0 \]  

with the correction function \( \beta \) from (13) and a function \( f \) that shows how the evolution of modes depends on an expanding background. Density perturbations obey a similar equation, but with a differently modified speed for inverse-triad corrections [110]. Interesting phenomenological effects are therefore suggested. (For holonomy corrections in currently existing versions, the modified speeds of density perturbations and gravitational waves are identical [112].)

Holonomy modifications at high density are especially drastic: they imply signature change [102, 113]. We are no longer dealing with quantum space-time but with a quantum version of four-dimensional Euclidean space, shown by the sign change of \( \beta(K) \) for large \( \ell K \). The deformed hypersurface-deformation algebra (13) then belongs to Euclidean-type space, and (104) shows the elliptic nature of linear mode equations. For positive as well as negative \( \beta \), we do not have standard space or space-time unless the value is exactly \( \pm 1 \); quantum space-time effects always occur. But the distinction between positive and negative values of \( \beta \), as opposed to two different positive values, is much more important because it changes the type of initial-value or boundary problems in mode equations. Signature change defined by the sign of \( \beta \) is therefore physically relevant, even in the absence of a standard classical space-time structure. In these high-density regimes, however, it is no longer consistent to treat holonomy corrections in isolation because they mix with quantum back-reaction, together forming higher-curvature corrections.

So far, no consistent deformation of the constraint algebra has been found for quantum corrections caused by quantum back-reaction, adding moment-dependent terms to the classical constraints. The problem is well-defined because we know the Poisson algebra of moments, and even though canonical effective field theory techniques remain incomplete, one could use those of quantum mechanical models in loop quantum gravity restricted to fixed graphs. In any finite region, there would then be a finite, though large, number of degrees of freedom given by link holonomies and plaquette fluxes. (Most calculations in the full theory are done with fixed graphs, anyway.) Since Poisson brackets of moments always produce other moments, quantum corrections must be arranged so that surplus terms delicately cancel in the constraint algebra.
No such version has been found yet, which is not altogether surprising because a successful implementation would imply a consistent version of quantum space-time, including moments of a state preserving covariance.

5.4. Anomaly problem

The problem of finding consistent deformations of the hypersurface-deformation algebra is related to the long-standing anomaly issue of canonical quantum gravity. If one can find an anomaly-free representation of quantum constraint operators, turning the classical constraint algebra into some operator version, effective constraints will automatically be first class and consistent: if two constraint operators $\hat{C}_1$ and $\hat{C}_2$ commute up to another constraint operator, the quantum constraints $\langle \hat{C}_1 \rangle$ and $\langle \hat{C}_2 \rangle$ Poisson commute up to another quantum constraint, thanks to $\{\langle \hat{C}_1 \rangle, \langle \hat{C}_2 \rangle\} = \langle [\hat{C}_1, \hat{C}_2] \rangle / i \hbar$. This statement also extends to higher-order quantum constraints $\langle f(\hat{q}, \hat{p}) \hat{C} \rangle$ [37].

Structure functions in the constraint algebra cause several problems in trying to find anomaly-free operator versions. But if such a version has been found, there are no additional problems in the transition to effective constraints. The product $[\hat{C}_1, \hat{C}_2] = f\hat{C}$ with a quantized structure function $f$ will, after taking an expectation value, be one of the higher-order quantum constraints. However, there are obstructions to simple attempts at solving the anomaly problem for constraint operators, related for instance to the interrelation of ordering and self-adjointness issues especially in the presence of structure functions [114]. If Hamiltonian constraint operators are self-adjoint, the commutator $[[\hat{H}[M], \hat{H}[N]] / i \hbar$ quantizing $[[\hat{H}[M], \hat{H}[N]]$ in (12) is self-adjoint too. But classically the bracket equals a product of the local diffeomorphism constraint $D_a$ with the structure function $q^{ab}$, two expressions that have a non-vanishing Poisson bracket because $q^{ab}$ is not diffeomorphism invariant. Any quantization of the product $q^{ab}D_a$ can then be self-adjoint and have a chance of agreeing with $[[\hat{H}[M], \hat{H}[N]] / i \hbar$ only if a symmetric ordering is used. But if one simply reorders ‘$\hat{q}^{ab}\hat{D}_a$’ symmetrically, a metric factor would come to lie to the right of the diffeomorphism constraint, and the product would no longer annihilate physical states. An anomalous version of the constraints would be obtained.

In an effective description, the situation is more manageable. First, one can use calculations of Poisson brackets instead of commutators of operators, even in the presence of quantum corrections and ordering choices. Moreover, quantum corrections may be suitably parameterized, to take into account different ordering choices, quantization ambiguities in the representation of inverse-triad and holonomy operators, and general classes of states in terms of their moments. One can compute Poisson brackets with ambiguity functions, such as (39), or moment terms unspecified, and see what conditions anomaly-freedom imposes on them. An operator calculation with free functions or states, by comparison, would be much more involved. The self-adjointness question can be left open at first by allowing for complex-valued constraints—kinematical moments appearing in effective constraints are complex-valued anyway, even in the absence of structure-function issues, as seen in section 4.1.5. With this strategy the first consistent deformations of the form (13) have been found [11], by now confirmed also by operator calculations [55]. The effective view is therefore reliable and powerful also in the context of the anomaly problem.

5.5. Quantum back-reaction and higher time derivatives

Moments and their quantum back-reaction, if they appear in a consistent deformation of the constraint algebra, are the canonical analog of higher-curvature terms with their higher time derivatives. However, their form is not directly one of higher time derivatives, and
additional steps and expansions, primarily an adiabatic one, are required to put canonical effective equations in the form of higher-derivative ones; see section 4.1.2. The adiabatic approximation is not always applicable. It serves well for anharmonic oscillators expanded around the harmonic vacuum with its constant moments. Moments of the anharmonic vacuum change, but only slowly, and can be treated adiabatically. Solving for moments order by order in the adiabatic expansion then shows how they are related to higher time derivatives of expectation values. The same statements hold true in quantum field theory, where one expands around the free vacuum in order to describe excitations around the interacting vacuum using the low-energy effective action.

These features have given rise to the expectation that quantum gravity should be subject only to higher-curvature corrections. However, two hidden assumptions are required for this conclusion. First, one assumes that quantum gravity implies corrections only in the dynamics of gravitons, say, not in the underlying space-time structure. Since gravity theories are fundamentally about space-time structure, this assumption, valid in a perturbative context of excitations on a fixed background, need not be true in general.

The second assumption is that quantum gravity can be realized perturbatively around some free theory of the usual form. Also this statement may be true for perturbations around a fixed background and perhaps some other situations, but it is not always valid. Quantum gravity is not expected to have a non-perturbative ground state, and other distinguished states may be very different from Gaussians as they appear in the harmonic-oscillator ground state or free vacuum states. Such states may not allow adiabaticity of the moments, and therefore cannot have a dynamics fully expressed by higher time derivatives. Indeed, examples in quantum cosmology are known in which the adiabaticity assumption is difficult to realize consistently [115]. Even for anharmonic oscillators, the adiabatic approximation is not valid when one perturbs around correlated coherent states, such as fully squeezed Gaussians, of the harmonic oscillator instead of the ground state [30, 70].

Instead of a higher-curvature or other higher-derivative effective theory, canonical quantum gravity has higher-dimensional effective systems in which the moments play the role of independent degrees of freedom in addition to expectation values. They are subject to their own equations of motion, and by quantum back-reaction couple to them, as e.g. in (46)–(50). Their effect can be formulated by higher-derivative terms only in certain regimes, but not in general.

5.6. Effective actions

So far, we have stayed in the canonical framework and dealt with effective equations and constraints. Complementary information can be obtained if a corresponding effective action is found. In principle, there is a one-to-one correspondence between canonical and Lagrangian formulations, but in perturbative settings, especially those that imply higher derivatives, the transformation is far from obvious. A derivative expansion of a Lagrangian may then correspond to a complicated resummation of a derivative-expanded Hamiltonian. It is therefore of interest to look for and study effective actions even if effective canonical equations are already known.

There are several examples in which effective actions have proven their usefulness in quantum cosmology. Euclidean path-integral techniques have been developed and applied to questions such as tunneling probabilities and some semiclassical issues [116–119]. As expected, in semiclassical regimes, corrections to Einstein’s equation are of higher-curvature form. Also causal dynamical triangulations have led to effective actions of cosmological systems by comparing detailed numerical studies of volume fluctuations with the dynamics of...
minisuperspace models [120]. By matching volume correlation functions with results expected from a higher-curvature effective action, quantum corrections can be derived. A general comparison involving also possible modifications to quantum space-time structure on top of higher-curvature corrections has not yet been completed. Effective actions of such forms often show more directly than other types of effective equations when quantum effects become significant.

Effective actions based on path integrals are subject to modified quantum space-time structures just as canonical effective equations and constraints. Path integration for gravitational theories requires an integration over all metrics, with a suitable measure that preserves covariance and does not introduce anomalies. Such a measure has not been found in complete generality, indicating that one encounters in this approach the same difficulties that appear when one tries to represent the canonical constraint algebra consistently. The path-integral measure is indeed the place to look at when one is interested in possible space-time modifications, but its incomplete nature does not give many clues. Canonical theories, with consistent deformations of the constraint algebra found in recent years, have been able to make more progress in this direction. (The spin-foam approach [121–123] attempts to take the results of loop quantum gravity regarding background-independent representations to a level comparable to path-integrals [124]. However, while some aspects of integrations over the space of metrics can be clarified, the issue of the correct measure, or spin-foam face amplitudes, remains open also here [125]. Notwithstanding these problems, traditional effective-action techniques have been applied to spin foams in [126].)

Another question in path-integral based approaches is how the state dependence enters effective actions. The low-energy effective action can be computed quite conveniently with path integrals, but it hides the fact that one is expanding around the ground state. If one tries to go beyond this limitation, which in quantum cosmology with its lack of ground states is a severe one, the required calculations become much more involved. Suitable states would have to be implemented by additional wave-function factors in the path integral, and integrations would no longer be Gaussian for general states. Moreover, since path integrals in their most common form provide transition amplitudes between two states separated by some finite time, one would have to put in the initial and final state. Compared to effective canonical equations, which only require initial moments to be specified, more a-priori information about the physical system is therefore required. In quantum cosmology, this information is not easily found by independent means, but is important for an analysis especially of the Planckian regime.

5.7. Regained dynamics: from canonical to Lagrangian

In this situation, a combination of canonical and Lagrangian effective methods is of interest. As already mentioned, it may be difficult to perform a transformation for constrained systems, especially those with higher-derivative terms. If the relation between the momenta and time derivatives of configuration variables involves higher derivatives, as easily happens with quantum-gravity corrections such as holonomy modifications, the Lagrangian would appear as a complicated resummation of the higher-derivative expansion of the Hamiltonian. Moreover, even if one can Legendre transform the Hamiltonian constraint to arrive at a Lagrangian, one would, for a comparison with path integrals, still have to look for a measure under which the modified Lagrangian is covariant. Also integrating the Lagrangian to an action requires new constructions even though just a classical measure on space-time is needed. However, with space-time structures modified and effective metrics non-existent—see section 5.3—defining
space-time integrations is non-trivial. Measure issues, therefore, cannot be resolved easily, but at least an effective Lagrangian for further classical-type analysis may still be found.

Instead of attempting a Legendre transformation, the canonical methods of [127, 128] can be used to derive a Lagrangian (or the constraints themselves) directly from a modified constraint algebra, to any given order in derivatives. If only second-order derivatives are assumed and the constraint algebra is classical, the Einstein–Hilbert action as a two-parameter family with Newton’s and the cosmological constant is obtained as the unique solution. If higher derivative orders are allowed, one expects higher-curvature corrections as well. And if even the constraint algebra is quantum corrected, as suggested by loop quantum gravity, stronger corrections, also to second derivative order, are obtained. With this procedure of ‘regaining’ a Lagrangian from the constraint algebra one can sidestep the complicated resummations that a Legendre transformation from modified constraints to the higher-derivative Lagrangian would imply. Not all coefficients in the Lagrangian may follow uniquely, especially if higher derivatives are included leaving several options of higher-curvature invariants of the same order. But the general form of modifications and implications for quantum space-time structure can still be found.

5.7.1. Functional equations. To spell out the general procedure, let us assume that we have a Hamiltonian or Hamiltonian constraint \( H(q, p) \) depending on canonical fields \( q(x) \) and \( p(x) \) in space. We introduce \( \delta H/\delta p =: v(x) \) as a new independent variable in place of \( p \), and then expand equations by this newly defined \( v \). If \( H \) is a Hamiltonian generating evolution in some fixed time parameter, we have \( v(x) = \dot{q}(x) \) by Hamilton’s equations. If \( H \) is a Hamiltonian constraint in the absence of an absolute time, \( v = (\delta N)^{-1}(q, H[\delta N]) \) is the derivative of \( q \) in a direction normal to spatial slices. For gravitational variables with \( q \) the metric or triad, \( v \) would therefore be related to extrinsic curvature. This change of variables amounts to what is needed for a Legendre transformation from \( (q, p) \) with Hamiltonian \( H \) to \( (q, v) \) with Lagrangian \( L = pv - H \), whose form will result as a solution of the \( v \)-expanded equations.

Note that we cannot always assume the Hamiltonian to be local and free of derivatives of \( p \), which would imply that partial derivatives could be used to compute \( v \). Holonomy corrections in loop quantum gravity, for instance, introduce higher spatial derivatives of the momentum conjugate to the densitized triad. In such situations, there is no local relation between the Hamiltonian and the Lagrangian, and explicitly performing a Legendre transformation is complicated.

Instead of computing the transformation, we intend to calculate the Lagrangian directly from the constraint algebra, assuming from now on the relations of the (deformed) hypersurface-deformation algebra. Using the definition of \( v \) and

\[
\frac{\delta H}{\delta q(x')} \bigg|_{p(x)} = - \frac{\delta L}{\delta q(x')} \bigg|_{v(x)}
\]

for the unsmeared Hamiltonian constraint and the Lagrangian density, we write the Poisson bracket (13) of two Hamiltonian constraints as

\[
\{H[N], H[M]\} = - \int d^3x \int d^3y \frac{\delta L(y)}{\delta q(x)} v(x)N(y)M(x) - \langle N \leftrightarrow M \rangle
\]

\[
= \int d^3x \beta D^a(x)(N\nabla_a M - M\nabla_a N)
\]

with the local diffeomorphism constraint \( D^a \). Taking functional derivatives by \( N \) and \( M \), we arrive at the functional equation

\[
\frac{\delta L(x)}{\delta q(x')} v(x') + \beta(x)D^a(x)\nabla_a \delta(x, x') - \langle x \leftrightarrow x' \rangle = 0
\]
for $L(x)$, which can be solved once an expression for the diffeomorphism constraint $D^a$ is inserted, depending on whether $q$ refers to gravity or some matter field. In all cases, $D^a$ is linear in the momenta. A linear equation for $L$ is thus obtained \([128]\). If \((10)\) and \((11)\) are unmodified, standard expressions for $D^a$ can be used. (See section 3.2 for a discussion of possible further modifications.)

5.7.2. Matter: To illustrate the regaining procedure, we look at a scalar matter field $\phi$ without derivative couplings, whose Hamiltonian obeys the (deformed) hypersurface-deformation algebra on its own, without adding the gravitational piece. The Lagrangian density must be of the form

$$L = \sqrt{\text{det} q} L(\phi, v, \psi)$$

where $v = (\delta N)^{-1}(\phi, H[\delta N])$, as before, is the normal scalar velocity and $\psi = q^{ab} \nabla_a \phi \nabla_b \phi$ is the only remaining scalar that can be formed from $\phi$ and its derivatives, to a total derivative order of at most two. Higher derivatives may easily result in interacting matter or quantum-gravity theories, with higher time derivatives from quantum back-reaction and higher spatial ones, additionally, from possible discretizations. (See e.g. \([129\text{--}132]\) for information about discretized space-time theories.) For now, however, we look for modifications implied by corrections that leave the classical derivative order unchanged.

With the canonical variables of a scalar field and its diffeomorphism constraint $D^a = p_\nu \nabla^\nu \phi$, equation \((108)\) assumes the form

$$\frac{\delta L(x)}{\delta \phi(x')} v(x') + \frac{\beta}{2} \frac{\delta L(x)}{\delta v(x')} (\nabla^a \phi(x')) \nabla_a \delta(x, x') - (x \leftrightarrow x') = 0. \quad (109)$$

As in \([128]\), we write

$$\frac{\delta L(x)}{\delta \phi(x')} = \frac{\delta L(x)}{\delta \phi(x)} \frac{\delta \phi(x)}{\delta \phi(x')} + 2 \frac{\partial L(x)}{\partial \psi(x')} (\nabla^a \phi(x')) \nabla_a \delta(x, x').$$

It follows that

$$A^a := (\nabla^a \phi) \left( \frac{\beta}{2} \frac{\partial L}{\partial v} + 2v \frac{\partial L}{\partial \psi} \right)$$

satisfies the equation $A^a(x) \nabla_a \delta(x, x') - (x \leftrightarrow x') = 0$, shown in \([128]\) to imply $A^a = 0$. Thus,

$$\beta \frac{\partial L}{\partial v} + 2v \frac{\partial L}{\partial \psi} = 0$$

and $L$ must be of the form $L(\phi, \psi - v^2/\beta)$. With non-trivial deformation, $\beta \neq 1$, the scalar field therefore obeys a modified dispersion relation. The kinetic term of the Lagrangian does not depend on $\psi - v^2 = g^{\mu\nu} (\nabla_\mu \phi)(\nabla_\nu \phi)$ in space-time terms, but has its time derivatives in $\psi - v^2/\beta$ rescaled by the correction function $\beta$. The resulting modified dispersion relation is in agreement with the wave equation \((104)\).

At the canonical level, for comparison, we begin with a matter Hamiltonian density of the form

$$H = v p_\phi^2 + \frac{1}{2} \sqrt{\text{det} q} \psi + \sqrt{\text{det} q} W(\phi) \quad (110)$$

with general inverse-triad correction functions $v$ and $\sigma$, and some potential $W(\phi)$. The corresponding Lagrangian density, with $v = v p_\phi/\sqrt{\text{det} q}$, takes the form

$$L = \sqrt{\text{det} q} \left( \frac{\psi^2}{2v} - \frac{\sigma \psi}{2} - W(\phi) \right) = -\sqrt{\text{det} q} \frac{\sigma}{2} \left( \psi - \frac{v^2}{\beta} \right) - \sqrt{\text{det} q} W(\phi). \quad (111)$$

This function has the same kinetic dependence as derived above, provided that $\beta = \nu \sigma$, exactly the requirement for an anomaly-free constraint algebra in the presence of inverse-triad corrections, where $\beta = \alpha^2$ \([11]\). Purely canonically, this consistency condition can be seen to ensure causality in the sense that gravitational waves on quantum space-time travel at the speed
of light, modified by a factor of $\sqrt{|\beta|}$ compared to the classical speed \[133\]. No super-luminal propagation happens when anomaly-freedom is taken into account, even if propagation speeds may be larger than the classical speed of light for $\alpha > 1$.

5.7.3. Effective action for inverse-triad corrections. For gravity, one example has been worked out in quite some detail with these methods: inverse-triad corrections of loop quantum gravity. These corrections have a characteristic component independent of higher derivatives, and therefore can be analyzed already at the level of second-order equations. The resulting second-order effective Lagrangian, regained from a modified constraint algebra with a correction function $\beta$ independent of curvature components, is

$$L_\beta = \frac{1}{16\pi G} \sqrt{\det q} \left( \frac{\text{sgn} \beta}{\sqrt{|\beta|}} (v_{ab} v^{ab} - v_a^a v_b^b) + \sqrt{|\beta|} (3R - 2\lambda) \right)$$

(112)

with ‘velocities’ $v_{ab}$, defined again as normal derivatives [102]. For classical gravity, $v_{ab} = 2K_{ab}$ would be proportional to extrinsic curvature. Compared with the classical action obtained for $\beta = 1$, the notion of covariance has changed: space and time derivatives are corrected by different coefficients $\sqrt{|\beta|}$ of $(3R)$ and $|\beta|^{-1/2}\text{sgn}(\beta)$ of $\frac{1}{4}(v_{ab} v^{ab} - v_a^a v_b^b)$, respectively. This result is consistent with the fact that the underlying constraint algebra is modified, taking the form (13). For this reason, as already mentioned in the context of line elements, the manifold structure required to integrate $L_\beta$ to an effective action is not clear. Nevertheless, the effective Lagrangian shows several characteristic effects. First, inverse-triad corrections, having implications even without higher-derivative or higher-order terms in $v_{ab}$, can easily be separated from holonomy effects and higher-curvature corrections. They are especially significant for small fluxes, where $\beta$ becomes small. With these constructions, it is possible to use inverse-triad corrections even when they imply strong modifications, regimes in which one would otherwise have to include full holonomy and higher-curvature corrections as well. These latter types of corrections are indeed present, but affect only higher orders in the $v$-expansion. Inverse-triad effects up to quadratic order in $v$ are reliable even if the other corrections are not known precisely.

Time derivatives are then dominant compared to the spatial Ricci scalar when $\beta$ approaches zero at small fluxes, indicating that near-singular geometries are controlled by homogeneous dynamics, strengthening the classical BKL scenario [134] by a no-singularity scenario in loop quantum gravity [135]. While holonomy effects cannot easily be seen at this level since they would manifest themselves only at higher orders in $v_{ab}$ and mix with higher-derivative terms, they have one drastic implication at high density if they are dominant. Then, the holonomy correction function $\beta$ becomes negative, a feature taken into account by the sign factors in (112). When the sign changes, the signature does too: at the Lagrangian level, one can interpret the effect by turning $t$ into $i t$ in (112) with $v_{ab}$ interpreted as first-order time derivatives. (The constraint algebra again provides a rigorous interpretation of this signature change; see section 5.2.) At Planckian densities, holonomy effects are so strong that they turn space-time into a quantum version of four-dimensional Euclidean space, lacking time and evolution. Temporal interpretations of high-density holonomy implications, such as bounces, are incorrect. Only large higher-derivative terms could prevent $\beta$ from turning negative, but then other holonomy effects such as bounces would go away too.

6. Implications for phenomenology and potential tests

It is difficult to test quantum cosmology by any observational means, and given the substantial lack of control over deep quantum regimes, devising high-density scenarios of the universe
remains a highly speculative exercise. Higher-curvature corrections, as they always appear in quantum gravity and cosmology except in the most simple harmonic models, are not relevant at currently accessible scales. They are certainly important in the Planckian regime, but then the present theories are so uncontrolled that it is impossible to derive clear effects, and even if some could be suggested, they would most likely be washed away by the immense amount of subsequent cosmic expansion.

If one goes beyond higher-curvature corrections as computed for Wheeler–DeWitt quantum cosmology in [136], using for instance quantum-geometry effects from loop quantum gravity, the situation has a chance of being more optimistic. Several investigations have been performed [137–145], but not all are based on consistent implementations of inhomogeneity. The general picture is therefore still incomplete. One type of corrections, holonomy modifications, provides contributions of higher powers of the connection or extrinsic curvature, very similar to some parts of higher-curvature corrections. Holonomy corrections therefore cannot be separated from higher-curvature effects, and cannot provide more-sizeable consequences regarding observations.

Moreover, the quantum space-time structure corresponding to holonomy corrections remains incompletely understood. Consistent deformations of the classical constraint algebra with some holonomy-like effects are known in spherically symmetric models [94, 95], 2 + 1-dimensional gravity [96] and for cosmological perturbations [93]. However, in spherically symmetric and cosmological models, only ‘pointwise’ holonomy modifications have been implemented, replacing connection components $c$ by $\exp(i \ell c)$ but not integrating over curves. Curve integrations, on the other hand, provide additional terms which are non-local or, when a derivative expansion (34) is used, introduce higher spatial derivatives. Keeping only higher powers of $c$ as in an expansion of the exponential, but ignoring spatial derivatives is not a consistent approximation: In strong curvature regimes, where holonomy effects should be significant, higher powers and higher derivatives of connection components both contribute to the same order of curvature.

Inverse-triad corrections, fortunately, are much better-behaved. First, the derivation of consistent deformations based on them is more complete, achieved in the same kind of models—cosmological perturbations [11], spherical symmetry [94, 95], and 2 + 1-dimensional models [55] in which operator calculations can be performed—but with all crucial terms included. Also inverse-triad corrections should come along with higher-derivative terms because they depend on fluxes, or integrated densitized triads. However, the non-derivative contribution is significant, as seen in section 5.7.3, and, unlike derivative terms, depends on parameters unrelated to curvature components. Moreover, additional derivative terms are included by the counterterms of [11], while no connection-derivative counterterms have been used for holonomy corrections in [93]. Inverse-triad corrections are therefore more reliable than holonomy corrections at the present stage of developments in loop quantum cosmology.

Inverse-triad corrections are also more interesting from an observational perspective. Because they do not directly refer to the curvature scale but rather to the discrete quantum-gravity scale related to the Planck length, there is no a-priori reason why they should be small at low curvature. They can play a role in standard cosmological scenarios, for instance during inflation. Indeed, in such a combined scenario, the window allowed for inverse-triad effects is much smaller than the one for curvature or holonomy modifications. For inverse-triad corrections, a parameter range of about four orders of magnitude is consistent with observations [59, 146], while curvature corrections have an allowed range of about ten orders of magnitude, one compared to the ratio of densities in observationally accessible regimes to the Planck density. There are also indications of interesting and characteristic effects in non-Gaussianity [147], although the required equations of motion second order in inhomogeneity
still have to be made consistent. By inverse-triad effects, loop quantum gravity becomes falsifiable.

For a more detailed review of phenomenological implications, see [148].

7. Outlook

Any quantum system can be evaluated consistently and reliably only when all possible quantum effects and the relevant degrees of freedom are taken into account. For quantum cosmology, this means that one must go beyond the traditional minisuperspace models and find consistent extensions to inhomogeneity. Quantum-representation issues then become much more involved, but can be handled for instance with methods of loop quantum gravity. In this canonical setting, a large set of effective techniques, described in the main part of this review, is now available. These methods allow one to forgo ad hoc assumptions, to implement full (but possibly deformed) space-time covariance, and to derive a complete phenomenological setting in which all relevant quantum effects are included. Unlike in traditional canonical quantizations and derivations of wave functions, there do not appear to be major obstacles on the way toward systematic comparisons with observations. Quantum cosmology is therefore empirically testable.

Concretely working out all terms and studying the necessary parameterizations of quantization and state ambiguities still remains to be completed. Even in isotropic models beyond the harmonic one, not much is known about the evolution of generic quantum states and the robustness of singularity avoidance (see sections 2.2 and 4). Control on inhomogeneous modes, necessary for most physical questions in cosmology and an understanding of quantum space-time, remains poor in strong quantum regimes, suffering from quantization ambiguities and the difficult anomaly problem (see sections 2.1 and 5). Effective techniques, especially effective constraints, have relieved some of the pressure caused by the failure of traditional methods to address these problems, but they have not been evaluated in sufficient detail to provide a reliable view on Planckian stages in cosmology. Further in-depth investigations are required to change this situation and to provide a complete and reliable phenomenology of quantum cosmology.

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