Chapter 4
Dynamics: Changing Atoms of Space–Time

In the previous chapter, we have seen some aspects of spatial quantum geometry, with its characteristic discrete spectra, emerge even in isotropic models. Now, these spatial structures have to fit into a consistent quantum space–time which in a certain sense reduces to a solution of Einstein's equation in a semiclassical or low-curvature limit. Only completing this most challenging step will make the theory one of quantum gravity, rather than of spatial quantum geometry.

4.1 Refinement and Internal Time

On general grounds, we expect discrete growth of the expanding universe in any theory with a microstructure of space–time. This has been anticipated several times [1, 2, 3] but never fully formulated. Loop quantum gravity makes progress at least in describing discrete spatial structures, and in providing means to analyze their evolution. A handle on these inhomogeneous features is necessary even for the consistency of the quantum cosmological theory: any kind of discreteness is in danger of being enlarged by the expansion of the universe and of becoming macroscopic unless its structure is being dynamically refined. It is not guaranteed that refinement happens in a suitable way so as to be consistent with the possibility of a macroscopic, very nearly continuous universe. Whether suitable refinement is realized can be checked in model systems, thereby providing feedback on the correct low-curvature limit of the full theory.

The picture we will take to develop dynamics is that of an evolving quantum geometry. Mathematically, it is implemented by constructing states in the Hilbert spaces seen before, but subject to the condition that they be annihilated by a quantization of the classical constraints: $\hat{C}|\psi\rangle = 0$. As the classical constraints make sure that initial data indeed are as they can be derived by restricting the geometry of a space–time solution to one of its spatial slices, quantum constraints ensure that there is no spurious gauge-dependent information in the quantum states we use. Discussing quantum constraints can be quite involved not just because the expressions

M. Bojowald, *Quantum Cosmology*, Lecture Notes in Physics 835,
DOI: 10.1007/978-1-4419-8276-6_4, © Springer Science+Business Media, LLC 2011

of constraints are complicated, but also because they are not always guaranteed to have zero as an eigenvalue in their discrete spectrum. In fact, especially for the Hamiltonian constraint of quantum gravity one expects interesting physical states to correspond to zeros in the continuous part of the spectrum. (There may be states in the discrete part as well.) Solutions then will not be normalizable in the spaces we constructed so far, and new inner products would have to be introduced to extract observable information from the states. Technical issues of constructing physical Hilbert spaces are discussed in Chap. 12.

Also the issue of observables strikes again: A general operator on the kinematical Hilbert space will not map a solution of $\hat{C}|\psi\rangle = 0$ to another such solution; it is guaranteed to do so only if it commutes with $\hat{C}$: $[\hat{O}, \hat{C}] = 0$. Such operators are called Dirac observables, and thanks to the commutation property they correspond to classical observables as phase-space functions invariant under the flow generated by the constraints: their classical correspondents satisfy $\{O, C\} = 0$. Unfortunately, complications in constructing general observables at the classical level become even more severe at the quantum level. For instance, one would have to be very careful with factor orderings to make a classical observable commute exactly with the constraints after quantization. (And exact commutation is required when it comes to removing gauge.)

We will discuss issues of physical Hilbert spaces and quantum observables in more detail in a later chapter; here we are primarily interested in the fact that the non-commutativity of the Hamiltonian constraint and operators for spatial geometry in general implies that physical states must be superpositions of different eigenstates of any operator of spatial geometry. Explicitly, this follows from the fact that the Hamiltonian constraint contains connection components, quantized to holonomies, which as creation operators excite the spatial geometry. No state with a sharp non-degenerate spatial geometry can be an eigenstate of such creation operators, and general superpositions are required.

Choosing a particular non-observable operator $\hat{\phi}$, for instance the volume or a matter field, and its eigenbasis, we expand a physical state as $|\psi\rangle = \sum_\phi |\psi\rangle_\phi$ where ϕ is a label for the eigenstates of $\hat{\phi}$. (Terms $|\psi\rangle_\phi$ in such a superposition are not physical states unless $\hat{\phi}$ is an observable.) We may then view the family $|\psi\rangle_\phi$ as an evolving quantum geometry, or a "state-time" [4]. It represents physical information, for it is just another way of writing the original physical state $|\psi\rangle$, supposed to solve the quantum constraint equation. Evolution is described not in coordinate time, as one usually does it in classical solutions, but with respect to an internal time ϕ. One could use a similar picture in classical gravity: The classical variable ϕ corresponding to the operator $\hat{\phi}$ we picked for the decomposition fulfills an equation of motion $\mathrm{d}\phi/\mathrm{d}t = \{\phi, C\} = f$ with some phase-space function f. At any phase-space point where $f \neq 0$, the usual t-derivatives in classical equations of motion can be traded for ϕ-derivatives by dividing all equations of motion by f. While such a procedure would usually make classical calculations more complicated than necessary, not even being too useful since one is mostly interested in the dependence of quantities on variables such as proper time, it is a more natural viewpoint to take in

quantum gravity. The quantum representation of geometry, after all, does not contain any space–time coordinates; it can refer only to degrees of freedom as found in the classical phase space, and so the internal-time picture is the only one available for evolution. Once physical states are parameterized with respect to an internal time, one can compute time-dependent expectation values of operators other than time $\hat{\phi}$ and their fluctuations or other moments. Even if such an operator $\hat{O}$ would not be an observable, the expectation value ${}_\phi\langle\psi|\hat{O}|\psi\rangle_\phi$ is meaningful. In general, however, care must be taken as to the inner product used here. For instance, one would like a sense of unitarity of ϕ-evolution to be realized, which then implies that ${}_\phi\langle\psi|\psi\rangle_\phi$ is constant in ϕ. (This is, of course, not guaranteed if the family $|\psi\rangle_\phi$ comes from an arbitrary decomposition of some state in any eigenbasis.)

Effective techniques allow one to formulate the concept of local internal time systematically, and to address the possible failure of unitarity of the evolution meaningfully. These methods and consequences such as the complexity of time will be discussed in Chap. 13; for now it suffices to know that consistent formulations can be provided, and we turn to the construction of the constraint operators themselves.

4.2 Constructions in the Full Theory

We will make use of the concept of internal time mainly in cosmological models where it is rather tractable. But we will first have to see what the Hamiltonian constraint and the dynamics it provides look like in the full theory, since this will be our guideline in reduced constructions just as it was for states and basic operators. Also for the dynamics, the key will be the use and form of holonomies, their appearance in the Hamiltonian constraint, and the way they influence superpositions in the averaging of kinematical to physical states. Remaining non-holonomy terms in the constraint are also important and provide clues to the small-scale behavior of quantum gravity, but they merely influence the concrete coefficients rather than the general form of such superpositions.

4.2.1 Gravitational Constraint

The classical expression of the Hamiltonian constraint in Ashtekar–Barbero variables is

$$C_{\mathrm{grav}}[N] = \frac{1}{16\pi\gamma G}\int_\Sigma \mathrm{d}^3x N\left(\varepsilon_{ijk}F^i_{ab}\frac{E^a_jE^b_k}{\sqrt{|\det E|}} - 2(1+\gamma^{-2})(A^i_a-\Gamma^i_a)(A^j_b-\Gamma^j_b)\frac{E^{[a}_iE^{b]}_j}{\sqrt{|\det E|}}\right) \tag{4.1}$$

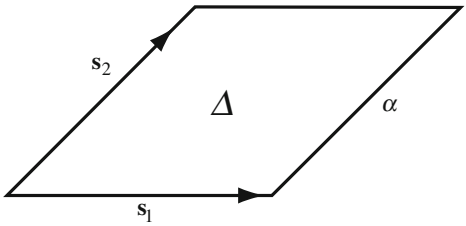

Fig. 4.1 A loop used to quantize curvature components

smeared with the lapse function N. As the main term responsible for the creation of geometrical excitations, we first turn to the curvature components F^i_{ab}. They are functionals of the connection components A^i_a, which in a loop representation cannot be quantized directly. Instead we have to use holonomies, providing curvature components via the well-known expression

$$s^a_1 s^b_2 F^i_{ab} \tau_i = \Delta^{-1}(h_\alpha - 1) + O(\Delta) \tag{4.2}$$

for the leading-order term of a holonomy along a closed loop α of square shape, of coordinate area Δ and along the tangent vectors s^a_1 and s^a_2; see Fig. 4.1.

The loop will give rise to holonomies and thus, when acting with the constraint, excitations of geometry [5]. There are different specific constructions, with different general behaviors. For instance, when acting on a given state the loop α may lie entirely on the graph of edges already excited for the state. In this case, the graph itself would not be changed, and no new vertices are being created (see e.g. [6]); only the excitation levels of existing edges are raised or lowered. Otherwise, if α does not lie entirely on the state's graph, new vertices and new edges will emerge [7]. In the picture of an evolving geometry, the number $\mathcal{N}$ of discrete sites may or may not change in the internal evolution parameter ϕ. But in all possible constructions put forward so far, individual sizes of elementary sites, earlier called v, must change: since the volume operator does not commute with all holonomies, $[\hat{V}, h] \neq 0$, vertex volumes of states must change in ϕ. While we do not yet have a systematic way of averaging these inhomogeneous results to isotropic geometries, the behavior seen here provides strong motivation for a lattice-refinement picture, and it does put limits on some parameters.

As the next important term in the classical constraint we have the triad-dependent function $\varepsilon^{ijk} E^b_j E^c_k / \sqrt{|\det E|}$. Fluxes cannot directly be used to quantize this expression since they have discrete spectra containing zero, making the determinant potentially degenerate. Instead, as already seen in the isotropic setting, one applies the classical identity [7]

$$\left\{ A^i_a, \int \sqrt{|\det E|} \mathrm{d}^3 x \right\} = 2\pi\gamma G \varepsilon^{ijk} \varepsilon_{abc} \frac{E^b_j E^c_k}{\sqrt{|\det E|}} \operatorname{sgn} \det(E^d_l) \tag{4.3}$$

(or another form since it is not unique) and quantizes the left-hand side regularly by using holonomies for A^i_a, the volume operator, and turning the Poisson bracket

into a commutator divided by $i\hbar$. A densely defined operator results. This key result of loop quantum gravity shows that Hamiltonians in quantum gravity, with similar constructions for matter Hamiltonians [8], can be made well-defined by particular properties of quantum geometry [7]. We do not have to normal-order Hamiltonian operators, which would be difficult in a background-independent way that lacks the ordinary creation and annihilation operators.[1] Coefficients in any superposition of physical states are automatically well-defined. In particular, the specific form of triad operators appearing in the constraint, containing commutators such as $h[h^{-1}, \hat{V}]$, changes vertices and their intertwiners for states they act on; thus another reason to expect a changing $v(\boldsymbol{\phi})$ in a physical state.

The remaining terms in the constraint are more difficult since they contain the spin connection (3.24), a complicated functional of E^a_i. Fortunately, they can be reduced to what has already been quantized by employing another Poisson identity [7]:

$$K^i_a = \gamma^{-1}(A^i_a - \Gamma^i_a) \propto \left\{ A^i_a, \left\{ \int \mathrm{d}^3x\, F^i_{ab} \frac{\varepsilon^{ijk} E^a_j E^b_k}{\sqrt{|\det E|}}, \int \sqrt{|\det E|}\mathrm{d}^3x \right\} \right\}. \quad (4.4)$$

Putting all these ingredients together, one constructs a well-defined Hamiltonian operator, schematically of the form

$$\hat{C}_{\mathrm{grav}}[N]\psi_g \propto \sum_{v\in V(g)} N(v) \sum_{e_I,e_J,e_K\in E(g)} \varepsilon^{IJK} \mathrm{tr}\left(h_I h_J h_K \left[h_K^{-1}, \hat{V}\right]\right) \psi_g \quad (4.5)$$

summing over vertices v and triples of edges $e_I \ni v$ of a graph g, with h_{IJ} the holonomy around a closed loop tangent to e_I and e_J in a vertex v. The specific form is subject to ambiguity, but the general form is characteristic and, as used later, easily extended to model systems.

There are several characteristic features implied by the construction steps, which give rise to corrections to the classical dynamics explored in quite some detail in this book. Also several fundamental properties arise in a specific form. For instance, for the resulting operator to be well-defined it is crucial that one orders the commutators quantizing inverse-triad components to the right of holonomies representing the curvature. When the commutator acts first on a cylindrical state, only vertex contributions appear. If holonomies act first, on the other hand, they create new vertices on arbitrary points of edges existing in the initial state, and on those new vertices (which are trivalent but not immediately gauge-invariant) the commutator has non-trivial action. Such an ordering would not give rise to a cylindrically consistent operator [7]. Once a consistent operator is defined, one may order it symmetrically by averaging with its adjoint. But this procedure is different from ordering the holonomies for curvature to the right [9]: for an operator creating new edges, as the Hamiltonian constraint does

[1] Notice that this sense of regularity does not by itself imply UV-finiteness in the usual meaning of quantum field theory. To test finiteness, one would have to compute scattering amplitudes of particle excitations on a quantum geometry state, which is difficult. It thus remains open how exactly a fundamentally finite version of loop quantum gravity could resolve non-renormalizability issues of perturbative quantum gravity.

by multiplying with holonomies, the adjoint removes edges. A symmetric ordering of such operators is different from simply reordering factors in its regularization.

The behavior of vertices under the action of the Hamiltonian constraint also plays a role for an argument of anomaly-freedom which one may make [10]. Commutators of Hamiltonian constraint operators should mimic the classical constraint algebra for the dynamics and gauge aspects to be consistent. (This theme will be discussed in more detail in the part on inhomogeneities, Chap. 10.) From the form of full Hamiltonian constraint operators one can argue that this is realized at least on diffeomorphism-invariant states, which are annihilated by the commutator. However, several difficulties with this very general statement arise: first, it has been pointed out that an extension to states that are not fully diffeomorphism invariant, and on which the off-shell constraint algebra should nevertheless be represented faithfully for anomaly-freedom, is difficult [11, 12]. Secondly, anomaly-freedom in the sense proposed in [10], even if it would work at a fundamental level, does not at all guarantee that effective geometries can be formulated with a consistent dynamics, a question which we will address later by other means. Thirdly, the same argument of anomaly-freedom does not apply in midisuperspace models such as spherically symmetric ones, see Chap. 9, whose vertex structure is different from the full one. While this failure of the argument may be due to a possible inadequacy of midisuperspace models regarding questions of fundamental anomaly-freedom, it should also be taken as a warning sign.

4.2.2 Matter Hamiltonian

Matter fields are quantized by similar means in a loop quantization, using graph states, and then coupled dynamically to the geometry by adding the matter Hamiltonian to the constraint. For a scalar field $\boldsymbol{\varphi}$, the density-weighted momentum $\pi = \sqrt{|\det E|}\dot{\boldsymbol{\varphi}}/N$ is a density of weight one. In the $\boldsymbol{\varphi}$-representation, states, as described in Sect. 3.2.2.3 will simply be of the form already used for the gravitational field, except that each vertex now also carries a label $\nu_v \in \mathbb{R}$ describing the dependence on the scalar field $\boldsymbol{\varphi}(v)$ through $\exp(\mathrm{i}\nu_v\boldsymbol{\varphi}(v))$ [13]. (The scalars take values in the Bohr compactification of the real line.) Well-defined lattice operators are given by $\widehat{\exp(\mathrm{i}\nu_0\boldsymbol{\varphi}(v))}$, for any $\nu_0 \in \mathbb{R}$, which shifts the label ν_v by ν_0. The momentum, with its density weight, has to be integrated before it can meaningfully be quantized. We introduce

$$P_R := \int_R \mathrm{d}^3x\pi$$

where R is a spatial region. Since we have $\{\boldsymbol{\varphi}(v), P_R\} = \chi_R(v)$ in terms of the characteristic function $\chi_R(v) = 1$ if $v \in R$ and zero otherwise, a momentum operator P_R has eigenvalue $\sum_{v\in R}\hbar\nu_v$ in a state introduced above.

For the matter Hamiltonian of a scalar field $\boldsymbol{\varphi}$ with momentum π and potential $W(\boldsymbol{\varphi})$ we have the classical expression

$$H_\varphi[N] = \int \mathrm{d}^3x N(x)\left(\frac{1}{2\sqrt{|\det E|}}\pi(x)^2 + \frac{E^a_i E^b_i}{2\sqrt{|\det E|}}\partial_a\boldsymbol{\varphi}(x)\partial_b\boldsymbol{\varphi}(x) + \sqrt{|\det E|}W(\varphi)\right)$$

containing inverse powers of the metric. It can be quantized by loop techniques [8, 14] making use of identities similar to (4.3). One first generalizes the identity to arbitrary positive powers of the volume in a Poisson bracket,

$$\{A^i_a, V^r_v\} = 4\pi\gamma G r V_v^{r-1} e^i_a \tag{4.6}$$

with V_v the volume of a small region including only the vertex v, and then combines such factors with suitable exponents r to produce a given product of triad and co-triad components. Since such identities would be used only when inverse components of densitized triads are involved and a positive power of volume must result in the Poisson bracket, the allowed range for r is $0 < r < 1$. Any such Poisson bracket will be quantized to

$$\dot{e}^a\{A^i_a, V^r_v\} \mapsto \frac{-2}{\mathrm{i}\hbar\delta}\mathrm{tr}\left(\tau^i h_{v,e}\left[h^{-1}_{v,e}, \hat{V}^r_v\right]\right) \tag{4.7}$$

using holonomies $h_{v,e}$ in direction $\dot{e}^a$, starting at v and of parameter length δ. These general parameterized expressions are also useful for alternative quantizations of terms in the gravitational part of the constraint, where different choices of r would represent quantization ambiguities.

The exponent used for the gravitational part is $r = 1$, while the scalar Hamiltonians introduced in [8, 14] use $r = 1/2$ for the kinetic term and $r = 3/4$ for the gradient term. With

$$\begin{aligned}\varepsilon^{abc}\varepsilon_{ijk}\{A^i_a, V_v^{1/2}\}\{A^j_b, V_v^{1/2}\}\{A^k_c, V_v^{1/2}\} &= (2\pi\gamma G)^3\varepsilon^{abc}\varepsilon_{ijk}\frac{e^i_a e^j_b e^k_c}{V_v^{3/2}}\\ &= 6(2\pi\gamma G)^3\frac{\det(e^i_a)}{V_v^{3/2}}\end{aligned}$$

and

$$\begin{aligned}\varepsilon^{abc}\varepsilon_{ijk}\{A^j_b, V_v^{3/4}\}\{A^k_c, V_v^{3/4}\} &= (3\pi\gamma G)^2\varepsilon^{abc}\varepsilon_{ijk}\frac{e^j_b e^k_c}{V_v^{1/2}}\\ &= 6(3\pi\gamma G)^2\frac{E^a_i}{V_v^{1/2}}\,\mathrm{sgn}\det(e^j_b)\end{aligned}$$

one can replace all inverse powers in the scalar Hamiltonian:

$$\hat{H}_\varphi[N]\psi_g = \sum_{v\in g} N(v)\left(\frac{1}{2}\hat{P}_v^2\left(\frac{1}{48}\sum_{e_I,e_J,e_K}\varepsilon^{IJK}\hat{B}^{(1/2)}_{v,e_I}\hat{B}^{(1/2)}_{v,e_J}\hat{B}^{(1/2)}_{v,e_K}\right)^2 + \frac{1}{2}\left(\frac{1}{48}\sum_{e_I,e_J,e_K}\varepsilon^{IJK}(\Delta_{e_I}\varphi)(v)\hat{B}^{(3/4)}_{v,e_J}\hat{B}^{(3/4)}_{v,e_K}\right)^2 + \hat{V}_v W(\varphi(v))\right)\psi_g \quad (4.8)$$

where $B^{(r)}_{v,e}$ denotes the vertex contribution at vertex v of a quantization of (4.7); $\Delta_e\boldsymbol{\varphi}$ denotes the difference operator along the edge e, and $\hat{P}_v$ is the vertex contribution to the momentum operator of the scalar.

In this way, inverse-triad corrections arise in matter Hamiltonians as well as in the gravitational part of the constraint, affecting the dynamics. What kind of effective action this might correspond to and whether these corrections can be consistent (not spoiling general covariance) will be discussed later in Chap. 10 about inhomogeneous perturbations. For now, we point out the relationship of full inverse-triad expressions based on (4.7) with the corresponding behavior in isotropic models. In isotropic models, we have seen that it is important to use the local patch volume V_v (as a power of the elementary fluxes F_{ℓ_0}) in order to ensure the correct scaling dependence. In (4.7), or the Hamiltonians (4.5) and (4.8), we could use V_v as well as the total volume V or that of any other region: volume contributions from vertices not lying on the edge used for holonomies in the commutator drop out, anyway. In homogeneous models, on the other hand, all vertices are equivalent and no such difference arises. It is then important to ensure that only local vertex contributions feature in the homogeneous expressions, which as seen in [15] has several other important implications regarding consistency.

4.2.3 Problem of Dynamics

Handling the dynamics is the key problem of any approach to quantum gravity. It splits into quite different but closely related subissues, the consistent construction of the dynamics on one hand, and the evaluation on the other. In isotropic quantum cosmology, the construction simplifies considerably and some of the key problems, such as that of anomalies, trivialize. One can thus focus on developing methods for the evaluation of quantum gravitational dynamics, which in the full setting has gained only preliminary insights. Important issues of the evaluation, which we will see in detail, are the role of lattice refinement, quantum back-reaction, and the implications of changing states. Later constructions in models including inhomogeneity will allow us to discuss also quantum space–time structure.

4.3 Isotropic Universes

A reduction of the Hamiltonian constraint from the full theory to symmetric models at the quantum level is difficult, but there is information about the reduction of states and spatial quantum geometry, as discussed in detail in Sects. 8.2.5, 9.1.3, and 10.1.2. This

formalism allows us to derive the basic quantum geometrical principles for isotropic loop quantum cosmology and then construct a Hamiltonian constraint operator along the lines used in the full theory. Since general spectral properties of basic operators, holonomies and fluxes, are preserved in this reduction, one can expect to capture important features of full loop quantum gravity at least at a qualitative level. Specific results seen in models can then be used to focus further derivations in the full theory.

4.3.1 Symmetry

Different procedures exist and are still being elaborated to reduce states from the full stage to a reduced setting [16–22]. A natural definition of a symmetric state is one that, as a functional on the space of connections, is supported only on the subset of invariant connections [16]. By this procedure, one can directly reduce any given state by evaluating it in the general expression of invariant connections for a symmetry type of interest, such as isotropy. The result will not be a spin network state, but rather a distribution on the full state space; it can be interpreted as being obtained by averaging an inhomogeneous state over the symmetry group. Such states are not embedded in the full Hilbert space but rather constitute truly reduced states. They comprise a minisuperspace quantization, but one obtained with input from the full theory. In contrast to Wheeler–DeWitt quantizations, crucial quantum space–time structures are still realized in the models derived in this way.

Suitable combinations of basic operators can then be found which map those states to others of this form, defining the basic representation of the model by reduction from the full holonomy-flux algebra. Difficulties arise when one tries to implement the full Hamiltonian constraint in such a way since it will not preserve the space of symmetric states, and projections to ensure this cannot easily be introduced at the distributional level. Constructions which may seem unnatural or contrived within a minisuperspace model but are required to incorporate full features thus remain required to implement the dynamics in a way mimicking the full one. No unique dynamics can result in this way, which even with a complete reduction would not be possible since the full dynamics is not unique in the first place. But with sufficiently general parameterizations one can explore the range of possibilities and extract general phenomena. As always with coarse-grained descriptions of microscopic physics, one has to suitably parameterize one's ignorance. If this is not done at a sufficiently general level, results will be spurious. No guidelines are provided in Wheeler–DeWitt quantizations, but much information is available from loop quantum gravity.

In particular, we will have to account for the crucial properties seen in the full theory. Every proposal for the full Hamiltonian constraint so far changes the individual sizes of discrete building blocks of geometry. In an isotropic setting this means that the function $\nu(\boldsymbol{\phi})$ in (2.16), now written in an internal time $\boldsymbol{\phi}$, must indeed be a function and cannot be constant in general. Although the precise form of $\nu(\boldsymbol{\phi})$ and the associated $\mathcal{N}(\boldsymbol{\phi})$ cannot easily be derived as mean fields of the refinement, a

quantization of isotropic dynamics must take the non-constant behavior of $v(\boldsymbol{\phi})$ into account in a sufficiently general way.

4.3.2 Models

Since holonomies are the basic operators exciting and refining the geometry, they will be crucial also in isotropic models. As already seen in Sect. 3.2.3.3, holonomies refer to the number $\mathcal{N} = \mathcal{V}/\ell_0^3$ of lattice states; now in a dynamical situation, $\mathcal{N}(\boldsymbol{\phi})$ will be a function of internal time. As in the full case, holonomies initially enter the Hamiltonian constraint via curvature components of the Ashtekar–Barbero connection, which in an isotropic setting reduces essentially to the Hubble parameter. Classically, we have a Hamiltonian constraint

$$C_{\mathrm{grav}} = -\frac{3}{8\pi G\gamma^2} c^2 \sqrt{|p|} + H_{\mathrm{matter}}(p, \varphi, p_\varphi) = 0 \tag{4.9}$$

written for simplicity only in the spatially flat case (and without curvature coupling in the matter Hamiltonian). Once the variables c and p are inserted in terms of the scale factor a, this constraint indeed gives rise to the Friedmann equation with energy density

$$\rho = \frac{H_{\mathrm{matter}}}{a^3 \mathcal{V}} \tag{4.10}$$

in terms of a matter Hamiltonian for the region of size $\mathcal{V}$.

The constraint also generates Hamiltonian equations of motion $\dot{f}(c, p) = \{f(c, p), C_{\mathrm{grav}}[N]\}$ for a general phase-space function f. To specify the choice of time coordinate, referred to by the dot, we have introduced the lapse function N, $C_{\mathrm{grav}}[N] = NC_{\mathrm{grav}}$. Its main choices usually are $N = 1$ for proper time and $N = a = \sqrt{|\tilde{p}|}$ for conformal time. Using the appearance of the lapse function in the canonical form of the metric, this indeed provides the correct isotropic line elements $\mathrm{d}s^2 = -\mathrm{d}t^2 + a^2\left(\mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2\right)$ in terms of proper time t, and $\mathrm{d}s^2 = a^2\left(-\mathrm{d}\eta^2 + \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2\right)$ in terms of conformal time η. Equations of motion for the basic variables read

$$\dot{p} = 2N\sqrt{|p|}c/\gamma, \tag{4.11}$$

implying the relationship $c = \mathcal{V}^{1/3}\gamma\dot{a}/N$ already seen, and

$$\dot{c} = \{c, C_{\mathrm{grav}}[N]\} = -\frac{c^2}{2\gamma\sqrt{|p|}}\left(N + 2p\mathrm{d}N/\mathrm{d}p\right) + \frac{8\pi\gamma G}{3}\frac{\partial H_{\mathrm{matter}}}{\partial p}. \tag{4.12}$$

This equation is the Raychaudhuri equation of the isotropic model, which can be brought to the standard form after using the thermodynamical relation

$$P = -\frac{\partial E}{\partial V} = -\frac{1}{3a^2\mathscr{V}N}\frac{\partial H_{\mathrm{matter}}}{\partial a} \tag{4.13}$$

for pressure. At this time, one should note that both equations, (4.11) and (4.12), are derived from the Hamiltonian constraint. When quantized, the Hamiltonian most likely receives quantum corrections, such that also these two equations, even the innocent-looking (4.11), will be corrected.

The classical Hamiltonian constraint is not directly representable in terms of holonomies due to the appearance of the non-almost periodic c^2. However, almost periodicity can be checked only when the full real range of the curvature variable c is taken, which includes arbitrarily large values of curvature where one would no longer trust the classical dynamics. At this time, the fundamental requirement that operators in an isotropic loop quantization must be representable through holonomies which are almost periodic in c becomes a guiding principle for deciding how the classical dynamics must change in quantum gravity. Restricting the function $c^2/p \propto (\dot{a}/a)^2$ to just a finite range, for instance up to Planckian curvatures, still allows one to extend it to an almost-periodic function in c over the full range. Such an extension is not unique, $\sin c$ and $\frac{1}{2}\sin(2c)$ being just two examples to extend c almost-periodically, but the resulting quantization ambiguity, as always, can be parameterized and then tested.

If we choose a class of almost-periodic extensions of c^2 by $\delta^{-2}\sin^2(\delta c)$ with a parameter δ, we can directly use the basic actions of $\exp(\mathrm{i}\delta c)$ and $\hat{p}$ to write the action of a Hamiltonian constraint operator. As expected from the presence of holonomies, it is a shift operator with terms raising and lowering the isotropic triad levels μ. Expanding a general state in the triad eigenbasis, $|\psi\rangle = \sum_\mu \psi_\mu|\mu\rangle$, we obtain the state's triad representation as the set of coefficients ψ_μ, which may also depend on other fields if different kinds of matter are present.

The construction proceeds along the following steps, which are analogous to those from the full theory but can now be performed very explicitly. We represent $\sqrt{|p|}$ via a commutator $e^{\mathrm{i}\delta c}\left[e^{-\mathrm{i}\delta c}, \hat{V}\right]$ to mimic the full treatment in the presence of inverse powers of the densitized triad. (In isotropic models the inverse powers cancel completely in the gravitational part of (4.9), and the treatment of inverse triads is not required at this stage. Crucial properties remain unchanged if one uses a more straightforward quantization of $\sqrt{|p|}$.) The action of the commutator on triad eigenstates follows as before for inverse-triad operators. Also the action of the holonomy term can be computed easily: $\sin^2(\delta c)$ maps $|\mu\rangle$ to $-\frac{1}{4}(|\mu+4\delta\rangle - 2|\mu\rangle + |\mu-4\delta\rangle)$. In the full theory, a consistent Hamiltonian constraint operator requires an ordering in which holonomies quantizing the curvature components F^i_{ab} appear to the left. Taking the same ordering in reduced models, we arrive at an operator with action

$$\hat{C}_{\mathrm{grav}}|\mu\rangle \propto \delta^{-3}\mathrm{sgn}(\mu)\left(V_{\mu+\delta} - V_{\mu-\delta}\right)(|\mu+4\delta\rangle - 2|\mu\rangle + |\mu-4\delta\rangle). \tag{4.14}$$

The constraint equation $\hat{C}_{\mathrm{grav}}|\psi\rangle = \hat{C}_{\mathrm{grav}}\sum_\mu \psi_\mu|\mu\rangle = \sum_\mu(\hat{C}_{\mathrm{grav}}\psi)_\mu|\mu\rangle = 0$ then implies a difference equation $(\hat{C}_{\mathrm{grav}}\psi)_\mu = 0$, of the form

$$\begin{aligned}&\mathrm{sgn}\,(\mu+4\delta)\left(V_{\mu+5\delta}-V_{\mu+3\delta}\right)\boldsymbol{\psi}_{\mu+4\delta}(\varphi)-2\mathrm{sgn}(\mu)\left(V_{\mu+\delta}-V_{\mu-\delta}\right)\boldsymbol{\psi}_{\mu}(\varphi)\\&+\mathrm{sgn}(\mu-4\delta)\left(V_{\mu-3\delta}-V_{\mu-5\delta}\right)\boldsymbol{\psi}_{\mu-4\delta}(\varphi)=-\frac{4}{3}\pi G\gamma^3\delta^2\ell_{\mathrm{P}}^2\hat{H}_{\mathrm{matter}}(\mu)\boldsymbol{\psi}_{\mu}(\varphi)\end{aligned}\tag{4.15}$$

for the wave function $\boldsymbol{\psi}_{\mu}(\varphi)$ in the triad representation. Its coefficients, written here in terms of volume eigenvalues $V_{\mu}=\left(4\pi\gamma\ell_{\mathrm{P}}^2|\mu|/3\right)^{3/2}$, follow from the representation of $\sqrt{|p|}$ as commutators.

The difference equation (4.15) follows from a constraint operator in which the commutator $h\left[h^{-1},\hat{V}\right]$ quantizing triad components is ordered entirely to the right of holonomies quantizing curvature components. This ordering is in fact suggested by the full theory as explained in Sect. 4.2.1. But once the operator has been defined, one can always order it symmetrically by replacing $\hat{C}_{\mathrm{grav}}$ with $\frac{1}{2}\left(\hat{C}_{\mathrm{grav}}+\hat{C}_{\mathrm{grav}}^{\dagger}\right)$. In this case coefficients of the difference equation change but the structure remains intact:

$$\begin{aligned}&\frac{1}{2}\left(\mathrm{sgn}(\mu+4\delta)\left(V_{\mu+5\delta}-V_{\mu+3\delta}\right)+\mathrm{sgn}(\mu)\left(V_{\mu+\delta}-V_{\mu-\delta}\right)\right)\boldsymbol{\psi}_{\mu+4\delta}(\varphi)\\&-2\mathrm{sgn}(\mu)\left(V_{\mu+\delta}-V_{\mu-\delta}\right)\boldsymbol{\psi}_{\mu}(\varphi)+\frac{1}{2}(\mathrm{sgn}(\mu)\left(V_{\mu+\delta}-V_{\mu-\delta}\right)\\&+\mathrm{sgn}(\mu-4\delta)\left(V_{\mu-3\delta}-V_{\mu-5\delta}\right))\boldsymbol{\psi}_{\mu-4\delta}(\varphi)\\&\quad=-\frac{4}{3}\pi G\gamma^3\delta^2\ell_{\mathrm{P}}^2\hat{H}_{\mathrm{matter}}(\mu)\boldsymbol{\psi}_{\mu}(\varphi).\end{aligned}\tag{4.16}$$

There are other ways to order an operator symmetrically, such as $\sqrt{\hat{C}_{\mathrm{grav}}^{\dagger}\hat{C}_{\mathrm{grav}}}$, but this would be more complicated to compute. One might also be tempted to define an operator symmetrically from the outset by splitting the $\sin^2(\delta c)$ in two factors to be positioned to the two sides of the commutator: $\sin(\delta c)h\left[h^{-1},\hat{V}\right]\sin(\delta c)$. (The commutator $h\left[h^{-1},\hat{V}\right]=\hat{V}-h\hat{V}h^{-1}$ automatically gives rise to symmetric operators when an su(2)-trace is taken.) However, this procedure does not properly mimic constructions in the full theory where h_{α} for a whole loop as in (4.2) could not be split into two equal factors.

Depending on the treatment of extrinsic-curvature contributions to the Lorentzian constraint (4.1), using (4.4), a difference equation of higher order than shown here may result. Such equations have been derived in [23, 24, 25].

4.3.3 Quantum-Geometry Corrections

In addition to obvious quantum features, two classes of quantum-geometry corrections are present: holonomy and inverse-triad corrections. Both of them are based directly on properties of the holonomy-flux algebra and the accompanying discreteness of space, but there is a difference in their realization. Inverse-triad corrections

result from a quantization of the classical reformulation (4.3) or (4.7) without regularization. Holonomy corrections, on the other hand, are obtained after replacing c^2 in the isotropic Hamiltonian constraint by some almost-periodic function approximated by c^2 when δc is small. After this modification of connection terms, the dynamics is no longer identical to the classical one. One may understand the higher-order terms as some of the contributions expected from higher-curvature effective actions,[2] but the modification is done at whim. It disappears in the classical limit only if $\delta \to 0$ in the classical limit, which requires one to relate the curve parameter to the Planck length. This relation, as seen in the context of lattice refinement, can be done only by reference to an underlying inhomogeneous state, not within the symmetric model; see Sect. 4.4.1.

The parameter δ is a regulator because it modifies the classical theory before it can be quantized by loop methods. Since the limit $\delta \to 0$ cannot be taken at the operator level—otherwise an operator for $\hat{c}$, not just for holonomies would exist—one must give the extra terms arising from the regularization some physical meaning. In loop quantum cosmology, this is done by interpreting them as higher powers of curvature which are not relevant for the small-curvature regime of the classical theory but are required for a well-defined quantum representation. At this stage, as always in loop quantizations, one takes a considerable risk: one assumes that the classical constraints can be modified in this way and still produce a reasonable theory. In particular covariance is at stake here, for one is adding only higher powers of the Ashtekar–Barbero connection at the Hamiltonian level, not higher powers of covariant curvature contractions at the level of an action. We will come back to the important related problem of anomalies later in this book (Chap. 10). For now, we notice that the key and still outstanding test of holonomy corrections is not to evaluate their dynamical implications in homogeneous models where they can be implemented freely, thanks to a trivialization of the anomaly problem, but rather a consistent extension to inhomogeneities.

In some models, notably isotropic ones with a free, massless scalar, it is possible to quantize the Hamiltonian constraint in exponentiated form, rather than exponentiating just the connection components [26]. One obtains an unregularized loop quantization without higher-order corrections. Such a quantization would be preferred compared to regulated ones because it would allow the anomaly-free inclusion of inhomogeneities in much simpler terms. It would also eliminate all holonomy effects. At the present stage of developments, however, the models in which such an unregulated loop quantization can be applied appear too special to rule out holonomy corrections altogether.

One can remove the regulator δ at the level of the difference equation provided one requires solutions to be smooth enough [27]. The difference equation then becomes a differential equation, essentially reproducing the Wheeler–DeWitt equation as the continuum limit. However, with the limit $\delta \to 0$ taken only at the level of

[2] These cannot be all contributions because higher-derivative terms of the metric do not arise by the holonomy replacement. See Chap. 13 for a general treatment of effective canonical dynamics which introduces new quantum degrees of freedom analogously to higher-derivative actions.

equations of motion for states, not in a full quantization, the resulting theory cannot be considered as fundamental.

It is sometimes suggested that the coordinate volume $\mathcal{V}$, which appears in δ but also in inverse-triad corrections, is a regulator and should be taken to infinity or the total size of a compact space. This is not correct because the classical theory simply does not depend on the value of $\mathcal{V}$. Sometimes in this context it is claimed that inverse-triad corrections disappear, just as holonomy corrections would disappear if the limit $\delta \to 0$ could be taken. Also here, the limit could only be taken at the level of equations, not at the level of operators where no inverse of the flux operator exists.

4.4 The Role of an Underlying State

So far, we have treated the parameter δ for different almost-periodic extensions as a constant. In a derivation of holonomies directly from isotropic connections in the general expression, we have $\delta = \ell_0/\mathcal{V}^{1/3}$ as seen earlier. In terms of the mean fields of lattice refinement, this can be written as $\delta = \mathcal{N}^{-1/3}$, which shows that a lattice-refinement model must be based on a parameter $\delta(\phi)$ depending on the internal time ϕ used to realize the refinement. In other words, while the size $\mathcal{V}$ is that of a constant region chosen once and for all to set up the quantization, the coordinate length ℓ_0 of curves used for holonomies can in general not be considered as a constant. Physically, the elementary discrete geometry must be refined during expansion to avoid that the discreteness scale is blown up to macroscopic sizes by the expanding universe. Such refinement indeed happens by a fundamental Hamiltonian constraint operator, which may generate new vertices and always changes the elementary sizes $v(\phi)$ of discrete building blocks.

In isotropic models, it is often convenient to use the scale factor a as internal time, such that we will have a function $\delta(a)$. In the mean-field picture, this will make the step-size δ of the difference equation dependent on the label μ: the equation is no longer one of constant step-size. We will later discuss how such equations can be dealt with; for now we are only interested in their general form.

4.4.1 Refinement Models

For specific difference equations based on refinement models, we would need $\mathcal{N}(a)$ or $v(a)$, related by $\mathcal{N}v = \mathcal{V}a^3$, as it arises from the genuine full dynamics in a suitable state. Lacking a derivation, we parameterize $\mathcal{N}(a) = \mathcal{N}_0 a^{-6x}$ such that $\delta(a) \propto a^{2x}$ and $v(a) = \mathcal{V}a^{3(1+2x)}/\mathcal{N}_0$. This is only an ansatz to probe different behaviors; in general $\mathcal{N}(a)$ need not be of power-law form for all a. But power-laws provide insights into the possible behaviors and can, at least for small ranges for a to vary, be used as approximations of general functions. Looking at different values of x, this procedure will show the behavior in different phases of refinement. For

$x > 0$, $\mathcal{N}$ is decreasing with expansion; for $x = 0$ it is constant and the discrete volume $v \propto a^3$ is proportional to the total volume. For $0 > x > -1/2$, both v and $\mathcal{N}$ are increasing, which makes it the regular range expected from the full behavior of the discrete dynamics.

Another, independent argument for $x < 0$ is that $\delta(a)$ then depends on a via a negative power, whose dimension can be compensated for only by a positive power of a parameter with dimension length. If the Planck length is used as this parameter, $\delta \to 0$ in the classical limit, removing holonomy corrections.

If $x = -1/2$, the local sizes v remain constant while the number $\mathcal{N}$ of sites increases proportionally to volume. As already seen, this behavior is unlikely from the point of view of the full theory because local vertex contributions to volume are always changed by the Hamiltonian constraint. It could at best be a coarse-grained, averaged description in a special case of the full dynamics. If $x < -1/2$, finally, the discrete sizes v must decrease when the universe expands. Since both $\mathcal{N}$ and v are bounded from below, the generic range where power-law behavior can be realized for long times is $-1/2 < x < 0$. Near the upper bound, however, the discrete volume contributions v are in danger of increasing too fast, or $\mathcal{N}$ is not increasing fast enough and refinement is too weak. In this regime, phenomenological restrictions on x can easily be found [28–32].

More generally, $\mathcal{N}$ may be a generic function, which one can think of as being composed of different power-law phases each parameterized by its own x. At this place we can see the real strength of using the Bohr compactification of the real line as kinematical quantum configuration space: for a single power-law form, the dynamical equation would always be periodizable by using $|p|^{1-x}$ instead of p as the state label, and $|p|^x c$ as the canonically conjugate curvature parameter in holonomies. Since the dynamics splits the range of all values into distinct sectors connecting only countably many values by the difference equation, we could from the outset have worked with states periodic in $\ell_0 \tilde{c} = c/\mathcal{N}^{1/3} \propto a^{2x} c$. Irrespective of whether we assume periodicity when choosing the dynamics or when formulating the kinematical states, such an assumption will always seem ad-hoc. If different power-laws or a non-power law function are involved, however, no periodicity occurs at all. This shows the real strength of the Bohr compactification by providing a repository for all possible refinement cases. (In a later chapter we will see that anisotropic models also make use of the full Bohr compactification without implicitly using periodic sectors, even if they are based on power-law behaviors of $\mathcal{N}$, crucially leading to non-equidistant difference equations.)

At this stage, it is worth commenting on differences between the mean-field picture and a pure minisuperspace quantization. We have first derived the constraint operator for a constant δ, and are then putting in the μ-dependence to ensure that full properties are reliably captured. One can also take the point of view that $\delta(p)$ is used from the outset, having to quantize a more complicated phase-space function $\exp(\mathrm{i}\delta(p)c)$ instead of ordinary holonomies. For simple choices of $\delta(p)$ of power-law form, such quantizations can be performed: one employs a canonical transformation such that the product $\delta(p)c$ which appears in the exponential is now one of the basic variables, and considers "holonomies" to be written in this variable. If

$\delta(p) \propto |p|^x$ is of power-law form, such a transformation can easily be done with $|p|^{1-x}$ being the new momentum conjugate to $|p|^x c$. For $x = -1/2$, for instance, this momentum would be the volume $V = |p|^{3/2}$. Pretending that $c/\sqrt{|p|}$ is to be used in almost-periodic holonomies would thus lead to a difference equation which is equidistant in volume values rather than densitized-triad values. For large μ, this procedure is equivalent to inserting $\delta(\mu) \propto |\mu|^{-1/2}$ directly in the basic difference equation (4.16), as one can see by substitution; for smaller μ, one can think of the equation obtained after a canonical transformation as providing one specific factor ordering of $\exp(\mathrm{i}\delta(p)c)$ which unlike the basic $\exp(\mathrm{i}\delta c)$ with constant δ is not defined uniquely. As one can see, however, there are difficulties in particular around $\mu = 0$ due to the absolute value used in fractional powers and the appearance of inverses of μ. Physically, this is not surprising since the μ-dependence of δ arises from lattice refinement, and around $\mu = 0$ not many lattice sites are excited. The lattice is thus very irregular, and one cannot expect to describe the behavior well by using simple power-laws for $\mathscr{N}(p)$. Keeping a general function $\delta(\mu)$ for basic properties of the dynamics, and specializing to simple forms only to analyze concrete cases at larger μ, is then the best way to shed light on the discrete dynamics.

Refinement is also relevant for inverse-triad operators and the corrections they imply, which contain the basic holonomies and fluxes (or the volume operator). In the commutator (4.7) used crucially in their definition, the local vertex volume V_v features, corresponding to the plaquette sizes in a refinement model.[3] As already discussed in Sect. 3.2.3.5, it is then not $p = \mathscr{V}^{2/3}a^2$ (the total box size) which features in commutators or correction functions but the plaquette size $\mathscr{N}^{-2/3}p = \ell_0^2 a^2$. This change makes the flux contribution, appearing as the argument of correction functions, smaller, and the correction correspondingly larger. For instance for $x = -1/2$ in a power-law form $\mathscr{N}(p)^{-1/3} = \delta(p) \propto |p|^x$, the plaquette size $\ell_0^2 a^2 = \mathscr{N}^{-2/3}|p|$ is constant. Large p do not make inverse-triad corrections shrink in this case, as it would happen without lattice refinement. Note that for a correct treatment of inverse-triad corrections with refinement, implemented by a phase-space dependent $\mathscr{N}(a)$, the refinement function is not to be inserted in the commutator before its computation, which would give the wrong result since the a-dependence of the factor would change the classical Poisson bracket. Refinement and the a-dependence is a mean-field effect, and thus to be inserted in the final expressions of an effective or coarse-grained theory. Since minisuperspace models by definition constitute coarse-grained descriptions of the full theory, mean-field treatments cannot be avoided altogether.

4.4.2 Interpretations

Different viewpoints have emerged in the development of loop quantum cosmology, all rooted in the original constructions of [23, 33–36]:

[3] In such commutators in the full theory, a single V_v gives the same contribution as the volume operator of all of space: contributions from vertices not lying on the edges used for the holonomy in the commutator cancel. But this observation does not change the fact that inverse-triad operators receive contributions only from local vertex contributions of the volume operator. In reduced models, homogeneity implies that all vertex contributions must contribute equally; one can properly capture the full behavior only by using single vertex or plaquette contributions from the outset.

Pure minisuperspace quantization[4]: One may argue that the curvature relation (4.2), $\delta^2 s_1^a s_2^b F^i_{ab}\tau_i \sim h_\alpha - 1$ with $h_\alpha \sim \sin^2(\delta c)$ in isotropic models, used crucially in quantizing the Hamiltonian constraint, should be evaluated by fixing the geometric area $A = a^2\delta^2$ as an ambiguity parameter rather than the coordinate area δ^2. If A indeed takes a fixed value, one obtains $\delta \propto 1/\sqrt{|p|}$, corresponding to the refinement scheme $x = -1/2$. In particular, by fixing A one trivially ensures that local patches of the underlying lattice state are constant, and thus $\mathscr{N} \propto \mathscr{V}$. (Most such realizations make use of the further ad-hoc assumption that this fixed value of A should be the minimal or some close-to-minimal non-zero eigenvalue of the full area spectrum. This condition is ad-hoc because it brings in the full area spectrum—the area operator in a reduced model does not have a non-zero minimal eigenvalue—and in that it crucially refers to the area operator at a place where it is not made use of in full constructions. Moreover, the resulting size of holonomy corrections is incompatible with inverse-triad corrections [15], implying an ℓ_0 that gives rise to large inverse-triad corrections even at large volume.)

The main (and perhaps only) justification of such a viewpoint toward the dynamics of loop quantum cosmology, compared to a constant δ, is a posteriori: A behavior of $\delta \propto 1/\sqrt{|p|}$ in holonomies appearing in the dynamics provides an additional suppression of higher powers of curvature at large volume, thus making it easier to comply with semiclassical and near-continuum behavior (provided inverse-triad corrections are ignored, which is often done in this context). Holonomy corrections depending on c^2/p rather than just c^2 are better behaved at large volume especially if there is a positive cosmological constant (in which case $c \propto \sqrt{|p|}$ at large volume is growing) or in the presence of intrinsic curvature. Moreover, holonomy corrections automatically depend on the scale-independent Hubble parameter $\dot{a}/a$. The pure minisuperspace viewpoint, without additional mean-field effects, thus presents a valid refinement scheme regarding curvature, but there are no strict arguments why it should be the preferred one. In fact, this viewpoint fails in Kantowski–Sachs models for the Schwarzschild interior, where a refinement with $\mathscr{N} \propto \mathscr{V}$ is not viable near the horizon; see Sect. 8.3. The scheme is also inconsistent with slow-roll inflation in the presence of inhomogeneities [39].

The starting point itself of the pure minisuperspace view is not fully convincing: curvature components F^i_{ab} are coordinate dependent, so why should one not refer to coordinate areas in their regularization? A reference to coordinates is indeed what happens in the full regularization, where using geometrical areas such as A would not be possible. Finally, the improved view in holonomies goes only half-way toward a consistent regularization. It uses refinement ideas in holonomies, where large-volume effects are potentially most problematic, but not for fluxes. Accordingly, minisuperspace quantizations typically produce wrong inverse-triad corrections by

[4] These models were initially introduced under the name "improved" quantization [37, 38], indicating advantages in certain regimes of low curvature and large volume. However, the modifications introduced in these models turned out to be rather ad-hoc. (To appreciate this realization, the models are sometimes called "improvised.") By now, what goes by the name "improved dynamics" is under strong pressure from different types of inconsistencies. The improved dynamics is itself to be improved, giving the name a rather misleading connotation.

overlooking the refinement for the volume operator appearing in commutators (see the Second Principle). In the pure minisuperspace context, it is then often stated erroneously that inverse-triad corrections play no role. By insisting that all quantum effects be realized in reduced operators, rather than partially in an underlying state, this view remains stuck in a mere minisuperspace picture, ignoring lessons from the full theory.

One undeniable advantage of the improved dynamics is that it removes ambiguities, if only by ad-hoc choices, and thus tends to provide very specific schemes and equations. For this reason, this special kind of the dynamics in loop quantum cosmology is often explored.

Refined loop quantum cosmology: A general and consistent viewpoint realizes that refinement is mainly implemented by properties of an underlying state: it is a mean-field effect that appears in minisuperspace models but crucially rests on behavior in the full theory. The incompleteness of the full theory and the complicated nature of symmetry reduction at the quantum level make it difficult to derive refinement models, but characteristic properties can be implemented by means of sufficiently general parameterizations; see Sect. 9.1.6.3 for a model that illustrates how refinement schemes could be derived. The state dependence will further be illustrated below. As the main justification for this refined view we state that it is required in general models such as black-hole interiors, and that only such a treatment can produce a consistent form of inverse-triad corrections.

4.4.3 Refinement from Reduction

Refinement arises in reduced models as a consequence of properties of underlying states used in the reduction. One may wonder why state-dependence should arise at all, and why effects cannot be captured completely in a reduction of operators. Properties of solutions to constraint equations certainly depend on the operators used, but the definition of reduced operators is normally not expected to depend on properties of $solutions$ to the full operator. And refinement, ultimately a consequence of the generation of new vertices or lattice sites by full Hamiltonian constraint operators, is a property of solutions to the full constraint equation.

If quantum cosmological models were fundamental, they should in fact be defined fully in terms of their operator algebra, and no free function such as $\mathcal{N}(p)$ or extra parameters such as $\mathcal{N}_0$ or x could appear. But quantum cosmological models are not fundamental; they provide an average description of full quantum gravity. In the averaging, additional features not captured fully by the operator algebra arise as mean fields.

A further crucial property especially in loop quantum gravity is the fact that regularizations of the full Hamiltonian constraint depend on the state the operator is going to act on. We refer to the graph when defining the loops used to rewrite the curvature components of the constraint. In the end, cylindrical consistency allows us to extend the graph-dependent definition to that of a consistent operator on the

full Hilbert space, but the state dependence of it remains. This state dependence can then reappear in reduced models in a way whose explicit details may be rather hidden by the reduction procedure but can still be parameterized. Such a reduction is complicated to do for the actual problem of interest, the Hamiltonian constraint operator of loop quantum gravity. But the resulting state dependence can easily be seen in an example:

Example 4.1 Consider a classical phase space with three canonical degrees of freedom $(q_1, p_1; q_2, p_2; q_3, p_3)$, subject to the first-class constraints $D = p_2$, $C = p_3$. Instead of performing a symmetry reduction, we are going to look at consequences of different implementations of gauge fixing the "diffeomorphism" constraint D, thus reducing the "Hamiltonian" constraint C. As the classical gauge-fixing condition we choose $F = q_2 - 1 = 0$.

Let us propose the state-dependent quantization (with regularization)

$$\hat{C}_{(n)} = \hat{p}_3 + 1 - \frac{\hat{q}_2^2 + \hat{p}_2^2}{2n+1}$$

on the subspace of the Hilbert space formed by states $\boldsymbol{\psi}_1 \otimes |n\rangle \otimes \boldsymbol{\psi}_3$ with $\left(\hat{q}_2^2 + \hat{p}_2^2\right)|n\rangle = (2n+1)|n\rangle$. By using any integer $n \geq 0$, a constraint operator with the correct classical limit is defined on the full Hilbert space. Note that the state-dependent regularization of $\hat{C}_{(n)}$ produces an anomalous quantization with $\left[\hat{D}, \hat{C}_{(n)}\right] = \hat{q}_2/(n+1/2) \neq 0$, resembling what may happen with the diffeomorphism and Hamiltonian constraint in loop quantum gravity.

If we simply implement the gauge-fixing conditions for D in a reduced setting, n becomes inaccessible. Just as we insert symmetric forms for the phase-space variables in a minisuperspace quantization, we would require $p_2 = 0$ and $q_2 = 1$ to implement $D = 0$ and $F = 0$ in a constraint operator $\hat{C}_{\mathrm{red}}$ for a reduced model, leaving us with the n-dependent

$$\hat{C}_{\mathrm{red},(n)} = \hat{p}_3 + 1 - \frac{1}{2n+1}.$$

We can recover n and thus uniquely fix the reduced Hamiltonian only if we know the state $|n\rangle$ that gives rise to the gauge fixing at the full quantum level, corresponding to the state of non-symmetric degrees of freedom in a minisuperspace quantization (the underlying state). At the state level, $p_2 = 0$ and $q_2 = 1$ is possible only for $n = 0$, which fixes n and brings the reduced Hamiltonian to the simple form $\hat{C} = \hat{p}_3$.

In this example, no trace of the state-dependent regularization is left if the reduction is done completely because no regularization of the operator was required in the first place; we just picked an unnecessarily contrived operator. For loop quantum gravity, the initial regularization and state dependence of the full Hamiltonian constraint is crucial, and so it should be expected to leave a trace in reduced models as well. It is also easy to see that the reduction parameters, as long as they are not eliminated by a complete reduction, may depend on the reduced or physical degrees

of freedom, just as a general refinement function $\mathscr{N}$ does. In the example here, we may regularize C to

$$\hat{C}_{(n)} = \hat{p}_3 + \left(1 - \frac{\hat{q}_2^2 + \hat{p}_2^2}{2n+1}\right)\hat{p}_1$$

and obtain a reduced Hamiltonian

$$\hat{C}_{\mathrm{red},(n)} = \hat{p}_3 + \left(1 - \frac{1}{2n+1}\right)\hat{p}_1$$

with a state-dependent correction depending on the physical observable $\hat{p}_1$.

In the preceding example, a full reduction, computing the exact state that implements the reduction condition, allowed us to arrive at a unique reduced Hamiltonian without any remnant of the state-dependent regularization. A further property that is realized in loop quantum gravity (the full diffeomorphism constraint relating symmetric and non-symmetric degrees of freedom) prevents this from happening, as a slight variation of the example shows:

Example 4.2 Now, take the constraints $D = p_2 + p_3$ with $C = p_3$ and the previous gauge-fixing condition $F = q_2 - 1 = 0$. Implementing $D = 0$ and $F = 0$ in a reduction with the same $\hat{C}_{(n)}$ as before then leads to the reduced Hamiltonian

$$\hat{C}_{\mathrm{red},(n)} = \hat{p}_3 + 1 - \frac{1 + \hat{p}_3^2}{2n+1}$$

and we are guaranteed a remnant of the state dependence in any reduced model: any value for n that may be obtained from a complete reduction can only depend on the (q_2, p_2)-state, and it cannot cancel the extra p_3 appearing in the reduced Hamiltonian.

As this set of examples shows, gauge-fixing the diffeomorphism constraint (for which symmetry reduction is one example), the regularization of the Hamiltonian constraint with its state dependence, and the anomaly issue all matter for a complete understanding of refinement. Currently, these issues are only poorly understood, and the best one can do is a sufficiently general parameterization of refinement options.

4.5 Basic Singularity Removal: Quantum Hyperbolicity

Given the difference equation in any form of lattice refinement, we use it to understand quantum evolution in the small-volume regime, near the singularity $\mu = 0$. First, in contrast to a Wheeler–DeWitt quantization based on metric variables and the scale factor a, the singular state is now in the interior of the configuration space rather than at a boundary: the freedom of having two possible orientations of the triad

makes μ take values of both signs. This fact opens up a direct way of testing whether there is a singularity in the sense of breakdown of evolution, since the difference equation for a state in the triad representation provides a natural evolution scheme via its recurrence. Irrespective of what internal time one would choose to describe evolution, that is whether it is indeed the triad value μ or something else entirely, we can test whether physical wave functions satisfying the constraint equation remain well-defined in a neighborhood of the singularity [40, 41].

Going through the recurrence, starting with suitable initial values on one side of positive μ, say, it is indeed easy to see, using (4.15) that $\mu = 0$ does not pose any obstruction. The matter Hamiltonian remains regular at $\mu = 0$, just as it does in the full theory at degenerate triads. Nevertheless, it could happen that the recurrence stops at $\mu = 0$ if coefficients of the difference equation vanish, preventing one from determining the next values of the wave function. For the form written here, coefficients can indeed vanish just at the classical singularity: for backward evolution toward smaller μ, the relevant term is $V_{\mu-3\delta(\mu)} - V_{\mu-5\delta(\mu)}$, which vanishes if $\mu = 4\delta(\mu)$. It multiplies $\boldsymbol{\psi}_0$, the value of the wave function at the classical singularity, which thus remains undetermined by initial data. This would be a disaster if that value would be required to continue the recurrence: the wave function at negative μ, "at the other side of the singularity," would not be determined by initial data at positive μ. At vanishing volume, evolution would still break down, and we would have a singularity as classically.

It turns out, however, that $\boldsymbol{\psi}_0$ is not needed for the further recurrence: it completely decouples from the rest of the wave function. Whenever it would show up in the difference equation, it is multiplied with a coefficient that vanishes at this rung of the ladder. (For the symmetric ordering of the constraint giving rise to the difference equation (4.16), we move through $\mu = 0$ without decoupling. Other orderings lead to singularities since $\boldsymbol{\psi}_0$ or other values of the wave function near $\mu = 0$ could not be determined but would be needed for further recurrence.) In this way, the recurrence can be undertaken through the place of the classical singularity; there is no singularity anymore and our evolving quantum space–time instead extends to a new region not seen classically. "Before" the big bang, in this internal-time picture and now back in forward evolution, we have a contracting universe since $V(\mu)$ decreases with increasing μ for $\mu < 0$. The change in sign of μ means that the orientation of the triad reverses in the big bang transition where the universe, as it were, turns its inside out.

Instead of determining the value of $\boldsymbol{\psi}_0$, the difference equation taken at $\mu = 4\delta(\mu)$ provides a linear equation for two values of the wave function that would be used in the recurrence for $\boldsymbol{\psi}_0$ if the $\boldsymbol{\psi}_0$-coefficient in the difference equation would not vanish. By the preceding recurrence steps, the linear equation can be traced back to one for the initial values chosen at some large μ, providing a dynamical initial condition [42, 43].

All this happens deeply in the quantum regime and different effects are at play. The difference-equation nature, crucial for the recurrence, relies on the use of holonomies. Comparing this to the classical expression of the constraint, we are considering higher-order corrections to the classically quadratic term in c, as it is

required for almost-periodic expressions. We also have crucially made use of the regular behavior of inverse-triad operators, especially in the matter Hamiltonian (which then annihilates $|0\rangle$). We have not specified a refinement scheme but just used the property that around $\mu = 0$, $\delta(\mu)$ is regular. Since singularity-traversal requires only a few μ-steps, possible changes in $\delta(\mu)$ can be ignored. The argument is independent of the refinement scheme. Finally, since we are considering the evolution of an entire wave function, there are implicit quantum back-reaction effects of the whole state on its expectation values, implying further deviations from classical evolution. All these effects are at play in the highly quantum phase around $\mu = 0$, which makes the development of an intuitive picture difficult. There are, however, simple special cases where one of the effects is dominant, or where the different effects can be separated from one another. Such models provide more intuitive pictures of at least some aspects of singularity resolution in loop quantum cosmology, and they allow one to develop effective descriptions, the topic of the next part.

References

1. Unruh, W.: Time, Gravity, and Quantum Mechanics pp. 23–94. Cambridge University Press, Cambridge (1997)
2. Weiss, N.: Phys. Rev. D **32**, 3228 (1985)
3. Jacobson, T.: (2000). hep-th/0001085
4. Bojowald, M., Singh, P., Skirzewski, A.: Phys. Rev. D **70**, 124022 (2004). gr-qc/0408094
5. Rovelli, C., Smolin, L.: Phys. Rev. Lett. **72**, 446 (1994). gr-qc/9308002
6. Giesel, K., Thiemann, T.: Class Quantum Grav. **24**, 2465 (2007). gr-qc/0607099
7. Thiemann, T.: Class Quantum Grav. **15**, 839 (1998). gr-qc/9606089
8. Thiemann, T.: Class Quantum Grav. **15**, 1281 (1998). gr-qc/9705019
9. Thiemann, T.: Class Quantum Grav. **15**, 875 (1998). gr-qc/9606090
10. Thiemann, T.: Phys. Lett. B **380**, 257 (1996). gr-qc/9606088
11. Lewandowski, J., Marolf, D.: Int. J Mod. Phys. D **7**, 299 (1998). gr-qc/9710016
12. Gambini, R., Lewandowski, J., Marolf, D., Pullin, J.: Int. J Mod. Phys. D **7**, 97 (1998). gr-qc/9710018
13. Ashtekar, A., Lewandowski, J., Sahlmann, H.: Class Quantum Grav. **20**, L11 (2003). gr-qc/0211012
14. Sahlmann, H., Thiemann, T.: Class Quantum Grav. **23**, 867 (2006). gr-qc/0207030
15. Bojowald, M.: Class Quantum Grav. **26**, 075020 (2009). arXiv:0811.4129
16. Bojowald, M., Kastrup, H.A.: Class Quantum Grav. **17**, 3009 (2000). hep-th/9907042
17. Engle, J.: Class Quantum Grav. **23**, 2861 (2006). gr-qc/0511107
18. Engle, J.: Class Quantum Grav. **24**, 5777 (2007). gr-qc/0701132
19. Koslowski, T.: (2006). gr-qc/0612138
20. Koslowski, T.: (2007). arXiv:0711.1098
21. Brunnemann, J., Fleischhack, C.: (2007). arXiv:0709.1621
22. Brunnemann, J., Koslowski, T.A. arXiv:1012.0053
23. Bojowald, M.: Class Quantum Grav. **19**, 2717 (2002). gr-qc/0202077
24. Hinterleitner, F., Major, S.: Phys. Rev. D **68**, 124023 (2003). gr-qc/0309035
25. Henriques, A.B.: Gen. Rel. Grav. **38**, 1645 (2006). gr-qc/0601134
26. Varadarajan, M.: Class Quantum Grav. **26**, 085006 (2009). arXiv:0812.0272
27. Bojowald, M.: Class Quantum Grav. **18**, L109 (2001). gr-qc/0105113
28. Nelson, W., Sakellariadou, M.: Phys. Rev. D **76**, 104003 (2007). arXiv:0707.0588

29. Nelson, W., Sakellariadou, M.: Phys. Rev. D **76**, 044015 (2007). arXiv:0706.0179
30. Grain, J., Barrau, A., Gorecki, A.: Phys. Rev. D **79**, 084015 (2009). arXiv:0902.3605
31. Grain, J., Cailleteau, T., Barrau, A., Gorecki, A.: Phys. Rev. D **81**, 024040 (2010). arXiv:0910.2892
32. Shimano, M., Harada, T.: Phys. Rev. D **80**, 063538 (2009). arXiv:0909.0334
33. Bojowald, M.: Class Quantum Grav. **17**, 1489 (2000). gr-qc/9910103
34. Bojowald, M.: Class Quantum Grav. **17**, 1509 (2000). gr-qc/9910104
35. Bojowald, M.: Class Quantum Grav. **18**, 1055 (2001). gr-qc/0008052
36. Bojowald, M.: Class Quantum Grav. **18**, 1071 (2001). gr-qc/0008053
37. Ashtekar, A., Pawlowski, T., Singh, P.: Phys. Rev. D **74**, 084003 (2006). gr-qc/0607039
38. Ashtekar, A., Wilson-Ewing, E.: Phys. Rev. D **79**, 083535 (2009). arXiv:0903.3397
39. Bojowald, M., Calcagni, G.: JCAP **1103**, 032 (2011). arXiv:1011.2779
40. Bojowald, M.: Phys. Rev. Lett. **86**, 5227 (2001). gr-qc/0102069
41. Bojowald, M.: Proceedings of the XIIth Brazilian School on Cosmology and Gravitation. In: AIP Conference Proceedings, vol. 910, pp. 294–333 (2007). gr-qc/0702144
42. Bojowald, M.: Phys. Rev. Lett. **87**, 121301 (2001). gr-qc/0104072
43. Bojowald, M.: Gen. Rel. Grav. **35**, 1877 (2003). gr-qc/0305069