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Lattice refining loop quantum cosmology, anisotropic models, and stability

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A general class of loop quantizations for anisotropic models is introduced and discussed, which enhances loop quantum cosmology by relevant features seen in inhomogeneous situations. The main new effect is an underlying lattice which is being refined during dynamical changes of the volume. In general, this leads to a new feature of dynamical difference equations which may not have constant step-size, posing new mathematical problems. It is discussed how such models can be evaluated and what lattice refinements imply for semiclassical behavior. Two detailed examples illustrate that stability conditions can put strong constraints on suitable refinement models, even in the absence of a fundamental Hamiltonian which defines changes of the underlying lattice. Thus, a large class of consistency tests of loop quantum gravity becomes available. In this context, it will also be seen that quantum corrections due to inverse powers of metric components in a constraint are much larger than they appeared recently in more special treatments of isotropic, free scalar models where they were artificially suppressed.

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I. INTRODUCTION

Loop quantum cosmology [1] was designed to test characteristic effects expected in the full framework of loop quantum gravity [2–4]. Implementing symmetries at the kinematical quantum level allows explicit treatments of the dynamical equations while preserving basic features such as the discreteness of spatial geometry [5]. (See also [6–11] for recent work on symmetry reduction in quantum theories.) Indeed, several new, initially surprising results were derived in different applications in cosmology and black hole physics. By now many such models have been studied in detail.

As the relation of dynamics to that of a possible full framework without symmetries is not fully worked out, detailed studies can be used to suggest improvements of the equations for physically viable behavior. Comparing results with full candidates for quantum dynamics can then provide stringent self-consistency tests of the overall framework. It is to be seen if, and how, such alterations of quantization procedures naturally result from a full quantization. The first example of this type related to the stability behavior of solutions to the difference equations of isotropic loop quantum cosmology, which was studied in [12,13] and was already restrictive for models with non-zero intrinsic curvature. Another limitation, realized early on [14], occurs in the presence of a positive cosmological constant Λ. In an exact isotropic model, the extrinsic curvature scale is given by $k = \dot{a} = \sqrt{8\pi G a^2 \Lambda/3}$ which, due to the factor of a^2, can be large in a late universe although the local curvature scale Λ might be small. Extrinsic curvature plays an important role since in a flat isotropic model it appears in holonomies on which loop quantizations are based in such a way that only $e^{i\alpha k}$ with $\alpha \in \mathbb{R}$ can be represented as operators, but not k itself [15]. Large values of k would either require one to use extremely small α in the relevant operators, or imply unexpected deviations from classical behavior. In fact, holonomies as basic objects imply that the Hamiltonian constraint is quantized to a difference rather than differential equation [16] since k in the Hamiltonian constraint (as in the Friedmann equation) is not directly quantized but only exponentials $e^{i\alpha k}$. These are shift operators instead of differential operators. For a large, semiclassical universe a Wheeler-DeWitt wave function should be a good approximation to the basic difference equation of loop quantum cosmology [17] which, in a representation as a function of the momentum $p = a^2$ conjugate to k, would be oscillating on scales of the order $(a\sqrt{\Lambda})^{-1}$. This scale becomes shorter and shorter in an expanding universe, eventually falling below the discreteness scale of the difference equation of loop quantum cosmology. At such a point, discreteness of spatial geometry would become noticeable in the behavior of the wave function (independently of how physical ob-

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servables are computed from it) although the universe should be classical.

This does not pose a problem for the general formalism, because it only shows that the specific quantization of the exact isotropic model used reaches its limits. Physically, this can be understood as a consequence of a fixed spatial lattice being used throughout the whole universe evolution. Exponentials $e^{i\alpha k}$ in isotropic models derive from holonomies $h_e(A) = \mathcal{P}\exp(\int_e A_a^i \tau_i \dot{e}^a \mathrm{d}t)$ of the Ashtekar connection along spatial curves e. All the freedom contained in choosing edges to capture independent degrees of freedom of the full theory reduces, in isotropic models, to the single parameter α which suffices to separate isotropic connections through all functions $e^{i\alpha k}$. The parameter α, from the full perspective, is thus related to the edge length used in holonomies. Using a fixed and constant α is analogous to using only edges of a given coordinate length, as they occur, for instance, in a regular lattice. In the presence of a positive cosmological constant, for any α a value of k will then be reached such that $e^{i\alpha k}$ differs strongly from $i\alpha k$. From the lattice perspective, this means that the local curvature radius becomes comparable to or smaller than the fixed lattice scale corresponding to α. Such a fixed lattice ceases to be able to support all small-scale oscillations relevant for a semiclassical geometry.

This is not problematic if it occurs in a quantum regime where dynamics is indeed expected to differ from the classical one, but it poses a problem in semiclassical regimes. A better treatment has to refer to changing lattices, which is not easy to implement in a straightforward quantization of purely homogeneous models. In a dynamical equation closer to what is expected from the full framework, lattice refinements would take place during the evolution since full Hamiltonian constraint operators generally create new vertices of a lattice state in addition to changing their edge labels [18–20]. While k increases with increasing volume, the corresponding α decreases since the lattice is being refined all the time. For a suitable lattice refinement, the increase in k can be balanced by the decrease of α such that αk stays small and semiclassical behavior is realized for any macroscopic volume even with $\Lambda > 0$. This provides an interesting relation between the fundamental Hamiltonian, which is responsible for the lattice refinement, and semiclassical properties of models. Testing whether an appropriate balance between increasing k and lattice refinements can be reached generically can thus provide stringent tests on the fundamental dynamics even without using a precise full Hamiltonian constraint operator.

This feature of lattice refinements was not mimicked in the first formulations of loop quantum cosmology [14,15,21–23] since the main focus was to understand small-volume effects such as classical singularities [24,25]. In this context, lattice refinements appear irrelevant because only a few action steps of the Hamiltonian, rather than long evolution, are sufficient to probe a singularity. By now, perturbative regimes around isotropic models have been formulated in loop quantum cosmology which are inhomogeneous and thus must take into account lattice states and, at least at an effective level, lattice refinements [9]. One special version, corresponding to lattices with a number of vertices growing linearly with volume in a specific way referring to the area operator, has been studied in detail in isotropic models with a free, massless scalar [26]. Although the complicated relation to a full, graph-changing Hamiltonian constraint is still not fully formulated, such models allow crucial tests of the local dynamics.

While isotropic models can easily be understood in terms of wave functions on a 1-dimensional discrete minisuperspace in terms of oscillation lengths [27], anisotropic models with higher-dimensional minisuperspaces can be more subtle. In such models, limitations similar to that of a cosmological constant have been observed as possible instabilities of solutions in classical regions or the lack of a sufficient number of semiclassical states [28–30]. For the partial difference equations of anisotropic models in loop quantum cosmology, stability issues can be much more severe than in isotropic models and thus lead to further consistency tests which might help to restrict possible quantization freedom (see, e.g., [31]). In this paper we therefore introduce the general setting of anisotropic models taking into account lattice refinements of Hamiltonian constraint operators, focusing mainly on the anisotropic model which corresponds to the Schwarzschild interior. As we will see, the type of difference equations in general changes since they can become nonequidistant. This leads to new mathematical problems which we address here briefly, leaving further analysis for future work. The examples presented here already show that one can distinguish different refinement models by their stability properties. The refinement model corresponding to [26] turns out to give unstable evolution of the Schwarzschild interior, while a new version, whose vertex number also grows linearly with volume, is stable. Compared to isotropic models which are sensitive only to how the vertex number of a state changes with volume, anisotropic models allow one to test much more detailed properties.

An appendix discusses subtleties in how homogeneous models faithfully represent inhomogeneous states, mainly regarding the magnitude of corrections arising from quantizations of inverse metric components which often plays a large role in cosmological applications.

II. DIFFERENCE EQUATION FOR THE SCHWARZSCHILD INTERIOR WITH VARYING DISCRETENESS SCALE

Basic variables of a loop quantization are holonomies along lattice links and fluxes over transversal surfaces. For the Schwarzschild interior [32], the connection used for

holonomies and the densitized triad used for fluxes take the form

$$A_a^i\tau_i \mathrm{d}x^a = \tilde{c}\tau_3 \mathrm{d}x + (\tilde{a}\tau_1 + \tilde{b}\tau_2)\mathrm{d}\vartheta + (-\tilde{b}\tau_1 + \tilde{a}\tau_2)\sin\vartheta \mathrm{d}\varphi + \tau_3\cos\vartheta \mathrm{d}\varphi \quad (1)$$

$$E_i^a\tau^i\frac{\partial}{\partial x^a} = \tilde{p}_c\tau_3\sin\vartheta\frac{\partial}{\partial x} + (\tilde{p}_a\tau_1 + \tilde{p}_b\tau_2)\sin\vartheta\frac{\partial}{\partial\vartheta} + (-\tilde{p}_b\tau_1 + \tilde{p}_a\tau_2)\frac{\partial}{\partial\varphi}. \quad (2)$$

Coordinates (x, ϑ, φ) are adapted to the symmetry, with polar angles ϑ and φ along orbits of the rotational symmetry subgroup, and $\tau_j = -\frac{i}{2}\sigma_j$ in terms of Pauli matrices. Spatial geometry is determined by the spatial line element, which in terms of the densitized triad components is

$$\mathrm{d}s^2 = \frac{\tilde{p}_a^2 + \tilde{p}_b^2}{|\tilde{p}_c|}\mathrm{d}x^2 + |\tilde{p}_c|\mathrm{d}\Omega^2 \quad (3)$$

obtained from $q^{ab} = E_i^aE_i^b/|\det E_j^c|$. We will also use the cotriad e_a^i, i.e., the inverse of $e_i^a = E_i^a/\sqrt{|\det E_j^b|}$,

$$e_a^i\tau_i \mathrm{d}x^a = e_c\tau_3\mathrm{d}x + (e_a\tau_1 + e_b\tau_2)\mathrm{d}\vartheta + (-e_b\tau_1 + e_a\tau_2)\sin\vartheta\mathrm{d}\varphi \quad (4)$$

with components

$$e_a = \frac{\sqrt{|\tilde{p}_c|}\tilde{p}_a}{\sqrt{\tilde{p}_a^2 + \tilde{p}_b^2}}, \qquad e_b = \frac{\sqrt{|\tilde{p}_c|}\tilde{p}_b}{\sqrt{\tilde{p}_a^2 + \tilde{p}_b^2}} \quad \text{and} \quad e_c = \frac{\mathrm{sgn}\tilde{p}_c\sqrt{\tilde{p}_a^2 + \tilde{p}_b^2}}{\sqrt{|\tilde{p}_c|}}. \quad (5)$$

The phase space is spanned by the spatial constants $(\tilde{a}, \tilde{b}, \tilde{c}, \tilde{p}_a, \tilde{p}_b, \tilde{p}_c) \in \mathbb{R}^6$ with nonvanishing Poisson brackets

$$\{\tilde{a}, \tilde{p}_a\} = \gamma G/L_0, \qquad \{\tilde{b}, \tilde{p}_b\} = \gamma G/L_0, \qquad \{\tilde{c}, \tilde{p}_c\} = 2\gamma G/L_0$$

where G is the gravitational constant and γ the Barbero-Immirzi parameter [33,34]. Moreover, L_0 is the size of a coordinate box along x used in integrating out the fields in

$$\frac{1}{8\pi\gamma G}\int \mathrm{d}^3x\dot{A}_a^iE_i^a = \frac{L_0}{2\gamma G}\dot{\tilde{c}}\tilde{p}_c + \frac{L_0}{\gamma G}\dot{\tilde{b}}\tilde{p}_b + \frac{L_0}{\gamma G}\dot{\tilde{a}}\tilde{p}_a$$

to derive the symplectic structure. The SU(2)-gauge transformations rotating a general triad are partially fixed to U(1) by demanding the x component of E_i^a to point in the internal τ_3 direction in (2). The U(1)-gauge freedom allows one to set $\tilde{a} = 0 = \tilde{p}_a$, still leaving a discrete residual gauge freedom $(\tilde{b}, \tilde{p}_b) \mapsto (-\tilde{b}, -\tilde{p}_b)$. The remaining variables can be rescaled by

$$(b, c) := (\tilde{b}, L_o\tilde{c}), \qquad (p_b, p_c) := (L_o\tilde{p}_b, \tilde{p}_c) \quad (6)$$

to make the canonical structure L_0-independent:

$$\{b, p_b\} = \gamma G, \qquad \{c, p_c\} = 2\gamma G. \quad (7)$$

This rescaling is suggested naturally by holonomies, as written below, and fluxes which are considered the basic objects in loop quantizations.

To express the elementary variables through holonomies, which unlike connection components will be promoted to operators, it suffices to choose curves along the x direction of coordinate length τL_0 and along ϑ of coordinate length μ since this captures all information in the two connection components,

$$h_x^{(\tau)}(A) = \exp\int_0^{\tau L_o}\mathrm{d}x\tilde{c}\tau_3 = \cos\frac{\tau c}{2} + 2\tau_3\sin\frac{\tau c}{2} \quad (8)$$

$$h_\vartheta^{(\mu)}(A) = \exp\int_0^{\mu}\mathrm{d}\vartheta\tilde{b}\tau_2 = \cos\frac{\mu b}{2} + 2\tau_2\sin\frac{\mu b}{2}. \quad (9)$$

The quantum Hilbert space is then based on cylindrical states depending on the connection through countably many holonomies, which can always be written as almost periodic functions $f(b, c) = \sum_{\mu,\tau}f_{\mu,\tau}\exp\frac{i}{2}(\mu b + \tau c)$ of two variables. These form the set of functions on the double product of the Bohr compactification of the real line, which is a compact Abelian group. Its Haar measure defines the inner product of the (nonseparable) Hilbert space, in which states

$$\langle b, c|\mu, \tau\rangle = e^{(i/2)(\mu b + \tau c)} \qquad \mu, \tau \in \mathbb{R} \quad (10)$$

form an orthonormal basis. Holonomies simply act by multiplication on these states, while densitized triad components become derivative operators

$$\hat{p}_b = -i\gamma\ell_{\mathrm{P}}^2\frac{\partial}{\partial b}, \qquad \hat{p}_c = -2i\gamma\ell_{\mathrm{P}}^2\frac{\partial}{\partial c} \quad (11)$$

using the Planck length $\ell_{\mathrm{P}} = \sqrt{G\hbar}$. They act as

$$\hat{p}_b|\mu, \tau\rangle = \frac{1}{2}\gamma\ell_{\mathrm{P}}^2\mu|\mu, \tau\rangle, \qquad \hat{p}_c|\mu, \tau\rangle = \gamma\ell_{\mathrm{P}}^2\tau|\mu, \tau\rangle, \quad (12)$$

immediately showing their eigenvalues.

To formulate the dynamical equation, one has to quantize the Hamiltonian constraint

$$H = \frac{1}{\gamma^2}\int \mathrm{d}^3x\epsilon_{ijk}(-\underline{F}_{ab}^k + \gamma^2\Omega_{ab}^k)\frac{E^{ai}E^{bj}}{\sqrt{|\det E|}} \quad (13)$$

where $\Omega_{ab}^k\tau_k\mathrm{d}x^a \wedge \mathrm{d}x^b = -\sin\vartheta\tau_3\mathrm{d}\vartheta \wedge \mathrm{d}\varphi$ is the intrin-

sic curvature of 2-spheres, while $\underline{F}^k_{ab}$ is the curvature computed from A^i_a ignoring the spin connection term $\sin\vartheta\tau_3 \mathrm{d}\varphi$. Following standard procedures a Hamiltonian constraint operator can be expressed in the basic operators. First, one replaces the inverse determinant of E^a_i by a Poisson bracket, following [19],

$$\epsilon_{ijk}\tau^i \frac{E^{aj}E^{bk}}{\sqrt{|\det E|}} = \frac{-1}{4\pi\gamma G} \sum_{K\in\{x,\vartheta,\varphi\}} \frac{1}{\ell_0^K} \epsilon^{abc}\omega_c^K h_K^{(\delta)}\{h_K^{(\delta)-1}, V\} \tag{14}$$

with edge lengths $\ell_0^x = \delta L_0$ and $\ell_0^{\vartheta/\varphi} = \delta$, and left-invariant 1-forms ω_c^K on the symmetry group manifold. For curvature components $\underline{F}^k_{ab}$ one uses a holonomy around a closed loop

$$\underline{F}^i_{ab}(x)\tau_i = \frac{\omega_a^I\omega_b^J}{\mathcal{A}_{(IJ)}}(h_{IJ}^{(\delta)} - 1) + O((b^2+c^2)^{3/2}\sqrt{\mathcal{A}}) \tag{15}$$

with

$$h_{IJ}^{(\delta)} = h_I^{(\delta)} h_J^{(\delta)} (h_I^{(\delta)})^{-1} (h_J^{(\delta)})^{-1} \tag{16}$$

and $\mathcal{A}_{IJ}$ being the coordinate area of the loop, using the corresponding combinations of ℓ_0^I. In these expressions, a parameter δ has been chosen which specifies the length of edges with respect to the background geometry provided by the symmetry group. Putting all factors together and replacing Poisson brackets by commutators, one has

$$\begin{aligned}\hat{H}^{(\delta)} &= 2i(\gamma^3\delta^3\ell_{\mathrm{P}}^2)^{-1}\,\mathrm{tr}\Big(\sum_{IJK}\epsilon^{IJK}\hat{h}_I^{(\delta)}\hat{h}_J^{(\delta)}\hat{h}_I^{(\delta)-1}\hat{h}_J^{(\delta)-1}\hat{h}_K^{(\delta)}[\hat{h}_K^{(\delta)-1},\hat{V}] + 2\gamma^2\delta^2\tau_3\hat{h}_x^{(\delta)}[\hat{h}_x^{(\delta)-1},\hat{V}]\Big)\\ &= 4i(\gamma^3\delta^3\ell_{\mathrm{P}}^2)^{-1}\Big(8\sin\frac{\delta b}{2}\cos\frac{\delta b}{2}\sin\frac{\delta c}{2}\cos\frac{\delta c}{2}\Big(\sin\frac{\delta b}{2}\hat{V}\cos\frac{\delta b}{2} - \cos\frac{\delta b}{2}\hat{V}\sin\frac{\delta b}{2}\Big)\\ &\quad + \Big(4\sin^2\frac{\delta b}{2}\cos^2\frac{\delta b}{2} + \gamma^2\delta^2\Big)\Big(\sin\frac{\delta c}{2}\hat{V}\cos\frac{\delta c}{2} - \cos\frac{\delta c}{2}\hat{V}\sin\frac{\delta c}{2}\Big)\Big)\end{aligned} \tag{17}$$

which acts as

$$\begin{aligned}\hat{H}^{(\delta)}|\mu,\tau\rangle = (2\gamma^3\delta^3\ell_{\mathrm{P}}^2)^{-1}[&2(V_{\mu+\delta,\tau} - V_{\mu-\delta,\tau})(|\mu+2\delta,\tau+2\delta\rangle - |\mu+2\delta,\tau-2\delta\rangle - |\mu-2\delta,\tau+2\delta\rangle\\ &+ |\mu-2\delta,\tau-2\delta\rangle) + (V_{\mu,\tau+\delta} - V_{\mu,\tau-\delta})(|\mu+4\delta,\tau\rangle - 2(1+2\gamma^2\delta^2)|\mu,\tau\rangle + |\mu-4\delta,\tau\rangle)]\end{aligned}$$

on basis states. This operator can be ordered symmetrically, defining $\hat{H}^{(\delta)}_{\mathrm{symm}} := \frac{1}{2}(\hat{H}^{(\delta)} + \hat{H}^{(\delta)\dagger})$, whose action is [35]

$$\begin{aligned}\hat{H}^{(\delta)}_{\mathrm{symm}}|\mu,\tau\rangle = (2\gamma^3\delta^3\ell_{\mathrm{P}}^2)^{-1}[&(V_{\mu+\delta,\tau} - V_{\mu-\delta,\tau} + V_{\mu+3\delta,\tau+2\delta} - V_{\mu+\delta,\tau+2\delta})|\mu+2\delta,\tau+2\delta\rangle\\ &- (V_{\mu+\delta,\tau} - V_{\mu-\delta,\tau} + V_{\mu+3\delta,\tau-2\delta} - V_{\mu+\delta,\tau-2\delta})|\mu+2\delta,\tau-2\delta\rangle\\ &- (V_{\mu+\delta,\tau} - V_{\mu-\delta,\tau} + V_{\mu-\delta,\tau+2\delta} - V_{\mu-3\delta,\tau+2\delta})|\mu-2\delta,\tau+2\delta\rangle\\ &+ (V_{\mu+\delta,\tau} - V_{\mu-\delta,\tau} + V_{\mu-\delta,\tau-2\delta} - V_{\mu-3\delta,\tau-2\delta})|\mu-2\delta,\tau-2\delta\rangle\\ &+ \frac{1}{2}(V_{\mu,\tau+\delta} - V_{\mu,\tau-\delta} + V_{\mu+4\delta,\tau+\delta} - V_{\mu+4\delta,\tau-\delta})|\mu+4\delta,\tau\rangle - 2(1+2\gamma^2\delta^2)(V_{\mu,\tau+\delta} - V_{\mu,\tau-\delta})|\mu,\tau\rangle\\ &+ \frac{1}{2}(V_{\mu,\tau+\delta} - V_{\mu,\tau-\delta} + V_{\mu-4\delta,\tau+\delta} - V_{\mu-4\delta,\tau-\delta})|\mu-4\delta,\tau\rangle].\end{aligned} \tag{18}$$

Transforming this operator to the triad representation obtained as coefficients of a wave function $|\psi\rangle = \sum_{\mu,\tau}\psi_{\mu,\tau}|\mu,\tau\rangle$ in the triad eigenbasis and using the volume eigenvalues

$$V_{\mu,\tau} = 4\pi\sqrt{|(\hat{p}_c)_{\mu,\tau}|}(\hat{p}_b)_{\mu,\tau} = 2\pi(\gamma\ell_{\mathrm{P}}^2)^{3/2}\sqrt{|\tau|}\mu,$$

a difference equation

$$\begin{aligned}\frac{\gamma^{3/2}\delta^3}{\pi\ell_{\mathrm{P}}}(\hat{H}^{(\delta)}_{\mathrm{symm}}|\psi\rangle)_{\mu,\tau} &= 2\delta(\sqrt{|\tau+2\delta|} + \sqrt{|\tau|})(\psi_{\mu+2\delta,\tau+2\delta} - \psi_{\mu-2\delta,\tau+2\delta})\\ &\quad + (\sqrt{|\tau+\delta|} - \sqrt{|\tau-\delta|})((\mu+2\delta)\psi_{\mu+4\delta,\tau} - 2(1+2\gamma^2\delta^2)\mu\psi_{\mu,\tau} + (\mu-2\delta)\psi_{\mu-4\delta,\tau})\\ &\quad + 2\delta(\sqrt{|\tau-2\delta|} + \sqrt{|\tau|})(\psi_{\mu-2\delta,\tau-2\delta} - \psi_{\mu+2\delta,\tau-2\delta}) = 0\end{aligned} \tag{19}$$

results for physical states. (For small μ the equation has to be specialized further due to the remaining gauge freedom; see [32]. This is not relevant for our purposes.)

A. Relation to fixed lattices

Although there are no spatial lattices appearing in the exactly homogeneous context followed here, the construction of the Hamiltonian constraint mimics that of the full theory. States are then associated with spatial lattices, and holonomies refer to embedded edges and loops. The parameter δ is the remnant of the loop size (in coordinates) used to act with holonomies on a spatial lattice. As one can see, this parameter is important for the resulting difference equation, determining its step-size. The above construction, using a constant δ, can be seen as corresponding to a lattice chosen once and for all such that the loop size is not being adjusted even while the total volume increases. As described in the introduction, this ignores the possible creation of new lattice vertices and links, and can be too rigid in certain semiclassical regimes.

To express this clearly, we now construct holonomies which are not simply along a single edge of a certain length δ, but which are understood as holonomies along lattice links. We keep our coordinate box of size L_0 in the x direction as well as the edge length ℓ_0. If this is a link in a uniform lattice, there are $\mathcal{N}_x = L_0/\ell_0$ lattice links in this direction, and a link holonomy appears in the form

$$h_x = \exp(\ell_0 \tilde{c}\tau_3) = \exp(\ell_0 c\tau_3/L_0) = \exp(c\tau_3/\mathcal{N}_x) \tag{20}$$

when computed along whole lattice edges. Thus, a constant coefficient $1/\mathcal{N}_x$ in holonomies corresponds to a fixed lattice whose number of vertices does not change when the volume increases. Lattice refinements of an inhomogeneous lattice state, on the other hand, can be mimicked by a parameter $\mathcal{N}_x$ which depends on the phase space variables, most important the triad components. If this is carried through, as we will see explicitly below, the step-size of the resulting difference equation is not constant in the triad variables anymore.

B. Lattice refinements

Let us now assume that we have a lattice with $\mathcal{N}$ vertices in a form adapted to the symmetry, i.e., there are $\mathcal{N}_x$ vertices along the x direction (whose triad component p_c gives rise to the label τ) and $\mathcal{N}_\vartheta^2$ vertices in spherical orbits of the symmetry group (whose triad component p_b gives rise to the label μ). Thus, $\mathcal{N} = \mathcal{N}_x\mathcal{N}_\vartheta^2$.

Since holonomies in such a lattice setting are computed along single links, rather than through all of space (or the whole cell of size L_0), basic ones are $h_x = \exp(\ell_0^x \tilde{c}\tau_3)$ and $h_\vartheta = \exp(\ell_0^\vartheta \tilde{b}\tau_2)$, denoting the edge lengths by ℓ_0^I and keeping them independent of each other in this anisotropic setting. Edge lengths are related to the number of vertices in each direction by $\ell_0^x = L_0/\mathcal{N}_x$ and $\ell_0^\vartheta = 1/\mathcal{N}_\vartheta$. With the rescaled connection components $c = L_0\tilde{c}$ and $b = \tilde{b}$ we have basic holonomies

$$h_x = \exp(\ell_0^x L_0^{-1} c\tau_3) = \exp(c\tau_3/\mathcal{N}_x), \tag{21}$$

$$h_\vartheta = \exp(\ell_0^\vartheta b\tau_2) = \exp(b\tau_2/\mathcal{N}_\vartheta). \tag{22}$$

Using this in the Hamiltonian constraint operator then gives a difference equation whose step-sizes are $1/\mathcal{N}_I$.

So far, we only reinterpreted δ in terms of vertex numbers. We now turn our attention to solutions to the Hamiltonian constraint which, in the full theory, usually changes the lattice by adding new edges and vertices while triad eigenvalues increase. For larger μ and τ, the Hamiltonian constraint thus acts on a finer lattice than for small values, and the parameter $\mathcal{N}$ for holonomies appearing in the constraint operator is not constant on phase space but triad dependent. Because of the irregular nature of lattices with newly created vertices such a refinement procedure is difficult to construct explicitly. But it is already insightful to use an effective implementation, using the derivation of the Hamiltonian constraint for a fixed lattice, but assuming the vertex number $\mathcal{N}(\mu, \tau)$ to be phase space dependent. Moreover, we include a parameter δ as before, which now takes a value $0 < \delta < 1$ and arises because a graph-changing Hamiltonian does not use whole lattice edges but only a fraction, given by δ [36]. Effectively assuming in this way that the lattice size is growing through the basic action of the Hamiltonian constraint, we will obtain a difference equation whose step-size $\delta/\mathcal{N}$ is not constant in the original triad variables.

For the Schwarzschild interior, we have step-sizes $\delta/\mathcal{N}_\vartheta$ for μ and $\delta/\mathcal{N}_x$ for τ. Going through the same procedure as before, we end up with an operator containing flux-dependent holonomies instead of basic ones, e.g., $\mathcal{N}_x(\mu, \tau)h_x = \mathcal{N}_x(\mu, \tau)\exp(c\tau_3/\mathcal{N}_x(\mu, \tau))$ which reduces to an $\mathcal{N}_x$-independent connection component c in regimes where curvature is small. Keeping track of all prefactors and holonomies in the commutator as well as the closed loop, one obtains the difference equation

$$\begin{aligned} &C_+(\mu, \tau)(\psi_{\mu+2\delta\mathcal{N}_\vartheta(\mu,\tau)^{-1},\tau+2\delta\mathcal{N}_x(\mu,\tau)^{-1}} - \psi_{\mu-2\delta\mathcal{N}_\vartheta(\mu,\tau)^{-1},\tau+2\delta\mathcal{N}_x(\mu,\tau)^{-1}}) \\ &\quad + C_0(\mu, \tau)((\mu + 2\delta\mathcal{N}_\vartheta(\mu, \tau)^{-1})\psi_{\mu+4\delta\mathcal{N}_\vartheta(\mu,\tau)^{-1},\tau} - 2(1 + 2\gamma^2\delta^2\mathcal{N}_\vartheta(\mu, \tau)^{-2})\mu\psi_{\mu,\tau} + (\mu - 2\delta\mathcal{N}_\vartheta(\mu, \tau)^{-1}) \\ &\quad \times \psi_{\mu-4\delta\mathcal{N}_\vartheta(\mu,\tau)^{-1},\tau}) + C_-(\mu, \tau)(\psi_{\mu-2\delta\mathcal{N}_\vartheta(\mu,\tau)^{-1},\tau-2\delta\mathcal{N}_x(\mu,\tau)^{-1}} - \psi_{\mu+2\delta\mathcal{N}_\vartheta(\mu,\tau)^{-1},\tau-2\delta\mathcal{N}_x(\mu,\tau)^{-1}}) = 0 \end{aligned} \tag{23}$$

with

$$C_{\pm}(\mu,\tau) = 2\delta\mathcal{N}_{\vartheta}(\mu,\tau)^{-1} \times (\sqrt{|\tau \pm 2\delta\mathcal{N}_x(\mu,\tau)^{-1}|} + \sqrt{|\tau|}),$$
$$C_0(\mu,\tau) = \sqrt{|\tau + \delta\mathcal{N}_x(\mu,\tau)^{-1}|} - \sqrt{|\tau - \delta\mathcal{N}_x(\mu,\tau)^{-1}|}. \quad (24)$$

(A total factor $\mathcal{N}_x\mathcal{N}_{\vartheta}^2$ for the number of vertices drops out because the right-hand side is zero in vacuum, but would multiply the left-hand side in the presence of a matter term.)

III. SPECIFIC REFINEMENT MODELS

For further analysis one has to make additional assumptions on how exactly the lattice spacing is changing with changing scales μ and τ. To fix this in general, one would have to use a full Hamiltonian constraint and determine how its action balances the creation of new vertices with increasing volume. Instead of doing this, we will focus here on two geometrically motivated cases. Technically simplest is a quantization where the number of vertices in a given direction is proportional to the geometrical area of a transversal surface. Moreover, the appearance of transversal surface areas is suggested by the action of the full Hamiltonian constraint which, when acting with an edge holonomy, creates a new vertex along this edge (changing $\mathcal{N}_I$ for this direction) and changes the spin of the edge (changing the area of a transversal surface). It also agrees with [26,37], although the motivation in those papers, proposing to use geometrical areas rather than coordinate areas $\mathcal{A}_{IJ}$ in (16), is different.

Geometrically more intuitive is the case where the number of vertices in a given direction is proportional to the geometrical extension of this direction [38]. The resulting difference equation will be more difficult to deal with due to its nonconstant step-size, but naturally gives rise to Misner-type variables. This case will also be seen to have improved stability properties compared to the first one using areas. In both cases, $\mathcal{N} \propto V$ is assumed, i.e., the lattice size increases proportionally to volume. This is not necessary in general, and we choose these two cases mainly for illustrative purposes. In fact, constant $\mathcal{N}$ as in [15] and $\mathcal{N} \propto V$ first used in [26] are two limiting cases from the full point of view, the first one without creating new vertices and the second one without changing spin labels along edges since local lattice volumes $V/\mathcal{N}$ remain constant. In general, both spin changes and the creation of new vertices happen when acting with a Hamiltonian constraint operator. Thus, one expects $\mathcal{N} \propto V^{\alpha}$ with some $0 < \alpha < 1$ to be determined by a detailed analysis of the full constraint and its reduction to a homogeneous model. Even assuming a certain behavior of $\mathcal{N}(V)$ without analyzing the relation to a full constraint leaves a large field to be explored, which can give valuable consistency checks. We will not do this systematically in this paper but rather discuss a mathematical issue that arises in any such case: initially, one has to deal with difference equations of nonconstant step-size which can be treated either directly or by tranforming a nonequidistant difference equation to an equidistant one. We first illustrate this for ordinary difference equations since partial ones, as they arise in anisotropic models, can often be reduced to this case.

A. Ordinary difference equations of varying step-size

Let us assume that we have an ordinary difference equation for a function ψ_{μ}, which appears in the equation with μ-dependent increments $\psi_{\mu+\delta\mathcal{N}_1(\mu)^{-1}}$. To transform this to a fixed step-size, we introduce a new variable $\tilde{\mu}(\mu)$ such that $\tilde{\mu}(\mu + \delta/\mathcal{N}_1(\mu)) = \tilde{\mu}(\mu) + \delta\tilde{\mu}'/\mathcal{N}_1(\mu) + O(\delta^2)$ has a constant linear term in δ. (For the isotropic equation, $\mathcal{N}_1$ is the vertex number only in one direction. The total number of vertices in a 3-dimensional lattice is given by $\mathcal{N} = \mathcal{N}_1^3$.) This is obviously satisfied if we choose $\tilde{\mu}(\mu) := \int^{\mu} \mathcal{N}_1(\nu)\mathrm{d}\nu$. We then have

$$\begin{aligned}\psi_{\mu+\delta/\mathcal{N}_1(\mu)} &= \tilde{\psi}_{\tilde{\mu}(\mu+\delta/\mathcal{N}_1(\mu))} \\ &= \tilde{\psi}_{\tilde{\mu}+\delta+\sum_{i=2}^{\infty}(1/i!)\delta^i\mathcal{N}_1^{(i-1)}/\mathcal{N}_1^i} \\ &= \tilde{\psi}_{\tilde{\mu}+\delta} + \frac{1}{2}\delta^2\frac{\mathcal{N}_1'}{\mathcal{N}_1^2}\tilde{\psi}' + O(\delta^3) \end{aligned} \quad (25)$$

where $\mathcal{N}_1^{(i)}$ denotes the i-th derivative of $\mathcal{N}_1$. Thus, up to terms of order at least δ^2 the new equation will be of constant step-size for the function $\tilde{\psi}_{\tilde{\mu}} := \psi_{\mu(\tilde{\mu})}$. (The derivative $\tilde{\psi}'$ by $\tilde{\mu}$ may not be defined for any solution to the difference equation. We write it in this form since such terms will be discussed below in the context of a continuum or semiclassical limit where derivatives would exist.)

It is easy to see that, for refining lattices, the additional terms containing derivatives of the wave function are of higher order in $\hbar$ and thus correspond to quantum corrections. For $\mathcal{N}_1(\mu) \propto \mu^q$ as a positive power of μ, which is the expected case from lattice refinements related to the increase in volume, we have

$$\frac{\mathcal{N}_1'}{\mathcal{N}_1^2} = \frac{q}{\mu\mathcal{N}_1(\mu)} = q\left(\frac{4\pi\gamma\ell_{\mathrm{P}}^2}{3p}\right)^{1+q}$$

relating μ to an isotropic triad component $p = 4\pi\gamma\ell_{\mathrm{P}}^2\mu/3$ as it occurs in isotropic loop quantum gravity [14]. Moreover,

$$\tilde{\psi}' = \frac{\mathrm{d}\tilde{\psi}}{\mathrm{d}\tilde{\mu}} = \frac{\mathrm{d}\mu}{\mathrm{d}\tilde{\mu}}\frac{\mathrm{d}\psi}{\mathrm{d}\mu} = \frac{1}{\mathcal{N}_1(\mu)}\frac{\mathrm{d}\psi}{\mathrm{d}\mu} = -\frac{i}{2}\frac{1}{\mathcal{N}_1(\mu)}\hat{c}\psi$$

in terms of a curvature operator $\hat{c} = 8\pi i\gamma G\hbar/3\mathrm{d}/\mathrm{d}p = 2i\mathrm{d}/\mathrm{d}\mu$ which exists in a continuum limit [17]. Thus,

$$\frac{\mathcal{N}_1'}{\mathcal{N}_1^2}\tilde{\psi}' \propto \left(\frac{\hbar}{p}\right)^{1+2q}\hat{c}\,\tilde{\psi}.$$

With q positive (or just larger than $-1/2$) for a refining lattice, there is a positive power of $\hbar$, showing that additional terms arising in the transformation are quantum corrections.

This has two important implications. First, it shows that the correct classical limit is obtained if lattices are indeed refined, rather than coarsened, since q is restricted for corrections to appear in positive powers of $\hbar$. In anisotropic models, as we will see, the behavior is more complicated due to the presence of several independent variables. An analysis of the semiclassical limit can then put strong restrictions on the behavior of lattices. Second, we can implicitly define a factor ordering of the original constraint giving rise to the nonequidistant difference equation by declaring that all quantum correction terms arising in the transformation above should cancel out with factor ordering terms. We then obtain a strictly equidistant equation in the new variable $\tilde{\mu}$. For example, a function $\mathcal{N}_1(\mu) = \sqrt{|\mu|}$ gives $\tilde{\mu} \propto |\mu|^{3/2}$ such that the transformed difference equation will be equidistant in volume rather than the densitized triad component. For this special case, factor orderings giving rise to a precisely equidistant difference equation have been constructed explicitly in [26,37].

B. Number of vertices proportional to transversal area

A simple difference equation results if the number of vertices is proportional to the square root of the transversal area in any direction [39]. In the x direction we have transversal surfaces given by symmetry orbits of area p_c, using the line element (3), and thus $\mathcal{N}_x \propto \sqrt{|\tau|}$. Surfaces transversal to a given angular direction, spanned by the x direction and the other angular direction, have area p_b, giving $\mathcal{N}_\vartheta \propto \sqrt{\mu}$. This way, the total number of vertices, $\mathcal{N}_x\mathcal{N}_\vartheta^2$, is proportional to the total volume. Each minisuperspace direction has a step-size which is not constant but independent of the other dimension. Moreover, due to the simple form one can transform the equation to constant step-size by using independent variables τ^2 and μ^2 instead of τ and μ. Illustrating the general procedure given before, a function $\tilde{\psi}_{\tau^{3/2},\mu^{3/2}}$ acquires constant shifts under the basic steps,

$$\begin{aligned}\tilde{\psi}_{(\tau+n\delta/\sqrt{\tau})^{3/2},(\mu+m\delta/\sqrt{\mu})^{3/2}} &= \tilde{\psi}_{\tau^{3/2}+(3/2)n\delta+\cdots,\mu^{3/2}+(3/2)m\delta+\cdots}\\ &= \tilde{\psi}_{\tau^{3/2}+(3/2)n\delta,\mu^{3/2}+(3/2)m\delta}\\ &\quad + O(\tau^{-3/2}) + O(\mu^{-3/2})\end{aligned}$$

up to terms which can be ignored for large τ and μ. This is sufficient for a straightforward analysis in asymptotic regimes. Moreover, higher order terms in the above equation come with higher derivatives of the wave function in the form

$$\frac{\tilde{\psi}'}{\tau^{3/2}} = \frac{\gamma^{3/2}\ell_{\mathrm{P}}^3}{p_c^{3/2}}\tilde{\psi}' \propto -i\frac{(\gamma\ell_{\mathrm{P}}^2)^2}{p_c^2}\hat{c}\,\tilde{\psi}$$

since $q = 1/2$ compared to the discussion in Sec. III A. Because of the extra factors of $\hbar$ (or even higher powers in further terms in the Taylor expansion) any additional term adding to the constant shift of $\tilde{\psi}_{\tau^{3/2},\mu^{3/2}}$ can be attributed to quantum corrections in a semiclassical limit. Accordingly, such terms can be avoided altogether by a judicious choice of the initial factor ordering of operators.

C. Number of vertices proportional to extension

Geometrically more intuitive, and as we will see below dynamically more stable, is the case in which the number of vertices in each direction is proportional to the extension of that direction measured with the triad itself. This gives $\mathcal{N}_\vartheta \propto \sqrt{|\tau|}$ and $\mathcal{N}_x \propto \mu/\sqrt{|\tau|}$, using the classical cotriad (4). (One need not worry about the inverse τ since the effective treatment of lattice refinements pursued here is not valid close to a classical singularity where an already small lattice with a few vertices changes. Singularities in general can only be discussed by a direct analysis of the resulting difference operators. Since only a few recurrence steps are necessary to probe the scheme around a classical singularity, equidistant difference operators are not essential in this regime. They are more useful in semiclassical regimes where one aims to probe long evolution times as in the examples below. Similar remarks apply to the horizon at $\mu = 0$ which, although a classical region for large mass parameters, presents a boundary to the homogeneous model used for the Schwarzschild interior.) The behavior is thus more complicated than in the first case since the step-size of any of the two independent variables depends on the other variable, too. First, it is easy to see, as before with quadratic variables, that the volume label $\omega = \mu\sqrt{|\tau|}$ changes (approximately) equidistantly with each iteration step which is not equidistant for the basic variables μ and τ. But it is impossible to find a second, independent quantity which does so, too. In fact, such a quantity $f(\mu, \tau)$ would have to solve two partial differential equations in order to ensure that

$$\begin{aligned}f(\mu + n\delta\mathcal{N}_\vartheta(\mu,\tau)^{-1}, \tau + m\delta\mathcal{N}_x(\mu,\tau)^{-1}) &\sim f(\mu,\tau)\\ &\quad + n\delta\mathcal{N}_\vartheta(\mu,\tau)^{-1}\partial_\mu f(\mu,\tau)\\ &\quad + m\delta\mathcal{N}_x(\mu,\tau)^{-1}\partial_\tau f(\mu,\tau)\end{aligned}$$

changes only by a constant independent of τ and μ. This implies $\partial_\mu f(\mu,\tau) \propto \sqrt{|\tau|}$ and $\partial_\tau f(\mu,\tau) \propto \mu/\sqrt{|\tau|}$ whose only solution is $f(\mu,\tau) \propto \mu\sqrt{|\tau|}$ which is the volume ω.

We thus have to deal with nonequidistant partial difference equations in this case which in general can be complicated. A possible procedure to avoid this is to split the iteration in two steps since an ordinary difference equation

can always be made equidistant as above (cancelling quantum corrections by reordering). We first transform τ to the volume variable ω which gives, up to quantum corrections, constant iteration steps for this variable. With the second variable still present, a higher order difference equation

$$C_0(\mu,\omega^2/\mu^2)(1+2\delta/\omega)\mu\psi_{\mu(1+4\delta/\omega),\omega+4\delta}+C_+(\mu,\omega^2/\mu^2)\psi_{\mu(1+2\delta/\omega),\omega+3\delta}-C_-(\mu,\omega^2/\mu^2)\psi_{\mu(1+2\delta/\omega),\omega+\delta}$$
$$-2C_0(\mu,\omega^2/\mu^2)(1+2\gamma^2\delta^2\mu^2/\omega^2)\mu\psi_{\mu,\omega}-C_+(\mu,\omega^2/\mu^2)\psi_{\mu(1-2\delta/\omega),\omega-\delta}+C_-(\mu,\omega^2/\mu^2)\psi_{\mu(1-2\delta/\omega),\omega-3\delta}$$
$$+C_0(\mu,\omega^2/\mu^2)(1-2\delta/\omega)\mu\psi_{\mu(1-4\delta/\omega),\omega-4\delta}=0 \quad (26)$$

results with

$$C_0(\mu,\omega^2/\mu^2)=\frac{\omega}{\mu}\left(\sqrt{1+\frac{\delta}{\omega}}-\sqrt{1-\frac{\delta}{\omega}}\right) \quad (27)$$

$$C_\pm(\mu,\omega^2/\mu^2)=2\delta\left(1+\sqrt{1\pm\frac{2\delta}{\omega}}\right) \quad (28)$$

derived from the original coefficients (24). The structure of this difference equation is quite different from the original one: not only is it of higher order, but now only one value of the wave function appears at each level of ω, rather than combinations of values at different values of μ. Note also that only the coefficient of the unshifted $\psi_{\mu,\omega}$ depends on μ. This form of the difference equation is, however, a consequence of the additional rotational symmetry and is not realized in this form for fully anisotropic Bianchi models as we will see below.

Proceeding with this specific case, we have to look at wave functions evaluated at shifted positions $\mu(1+m\delta/\omega)$ with integer m. At fixed $\omega=\omega_0$, we are thus evaluating the wave function at values of μ multiplied with a constant, instead of being shifted by a constant as in an equidistant difference equation. This suggests to use the logarithm of μ instead of μ itself as an independent variable, which is indeed the result of the general procedure. After having transformed from τ to ω already, we have to use τ as a function of μ and ω in the vertex number $\mathcal{N}_\vartheta$, which is $\tau(\mu,\omega)=(\omega/\mu)^2$ after using $\omega=\mu\sqrt{\tau}$. Thus, $\mathcal{N}_\vartheta(\mu,\tau(\mu,\omega))=\sqrt{\tau(\mu,\omega)}=\omega/\mu$ is no longer a positive power of the independent variable μ, and we will have to be more careful in the interpretation of correction terms after performing the transformation. (The lattice is coarsened with increasing anisotropy at constant volume.) Naively applying the results of Sec. III A to $q=-1$ would suggest that corrections come with inverse powers of $\hbar$ which would certainly be damaging for the correct classical limit. However, the factors change due to the presence of the additional variable ω_0 even though it is treated as a constant. We have $\mathcal{N}'_\vartheta/\mathcal{N}^2_\vartheta=-1/\omega_0=-(\gamma\ell_{\rm P}^2/2)^{3/2}/V_0$ in terms of the dimensionful volume V, while it would just be a constant -1 without the presence of ω. The additional factor of $\hbar^{3/2}$ ensures that corrections come with positive powers of $\hbar$ for the correct classical limit to be realized.

For any ω_0, we thus transform $\tilde{\psi}_{\mu(1+m\delta/\omega_0)}$ to equidistant form by using $\tilde{\tilde{\psi}}_{\tilde{\mu}}=\tilde{\psi}_{\mu(\tilde{\mu})}$ with $\tilde{\mu}(\mu)=\log\mu$. This transformation is possible since the second label ω_0 is now treated as a constant, rather than an independent variable of a partial difference equation. (Recall that for the type of difference equation discussed here there is only one variable, the volume, which is equidistant under all of the original discrete steps.) Despite negative powers of some variables in the vertex numbers, we have the correct classical limit in the presence of ω. As before, the transformation is exact up to higher order terms which are quantum and higher order curvature corrections. Defining the original constraint operator ordering implicitly by the requirement that all those terms are cancelled allows us to work with an equidistant difference equation.

D. Bianchi models

As mentioned before, the transformed difference equation does not become higher order for fully anisotropic Bianchi models. In this case, we have three independent flux labels μ_I, $I=1,2,3$, and vertex numbers $\mathcal{N}_I$. Using vertex numbers proportional to the spatial extensions for each direction gives $\mathcal{N}_1=\sqrt{\mu_2\mu_3/\mu_1}$, $\mathcal{N}_2=\sqrt{\mu_1\mu_3/\mu_2}$, and $\mathcal{N}_3=\sqrt{\mu_1\mu_2/\mu_3}$. As in the difference equation for the Schwarzschild interior, the difference equation for Bianchi models [23] uses values of the wave function of the form $\psi_{\mu_1+2\delta/\mathcal{N}_1,\mu_2+2\delta/\mathcal{N}_2,\mu_3}$. One can again see easily that the volume $\omega=\sqrt{|\mu_1\mu_2\mu_3|}$ behaves equidistantly under the increments,

$$\begin{aligned}&\omega(\mu_1+2\delta/\mathcal{N}_1,\mu_2+2\delta/\mathcal{N}_2,\mu_3)\\&=\sqrt{\left(\mu_1+2\delta\sqrt{\frac{\mu_1}{\mu_2\mu_3}}\right)\left(\mu_2+2\delta\sqrt{\frac{\mu_2}{\mu_1\mu_3}}\right)\mu_3}\\&=\sqrt{\mu_1\mu_2\mu_3+4\delta\sqrt{\mu_1\mu_2\mu_3}+4\delta^2}\\&=\omega+2\delta+O(\delta^2).\end{aligned}$$

The leading order term of the difference equation in ω results from a combination

$$C_1\psi_{\mu_1,\mu_2+2\delta/\mathcal{N}_2,\mu_3+2\delta/\mathcal{N}_3} + C_2\psi_{\mu_1+2\delta/\mathcal{N}_1,\mu_2,\mu_3+2\delta/\mathcal{N}_3} + C_3\psi_{\mu_1+2\delta/\mathcal{N}_1,\mu_2+2\delta/\mathcal{N}_2,\mu_3}$$
$$\approx C_1\tilde{\psi}_{\mu_1,\mu_2+2\delta/\mathcal{N}_2,\omega+2\delta} + C_2\tilde{\psi}_{\mu_1+2\delta/\mathcal{N}_1,\mu_2,\omega+2\delta} + C_3\tilde{\psi}_{\mu_1+2\delta/\mathcal{N}_1,\mu_2+2\delta/\mathcal{N}_2,\omega+2\delta}$$
$$= C_1\tilde{\psi}_{\mu_1,\mu_2(1+2\delta/\omega),\omega+2\delta} + C_2\tilde{\psi}_{\mu_1(1+2\delta/\omega),\mu_2,\omega+2\delta} + C_3\tilde{\psi}_{\mu_1(1+2\delta/\omega),\mu_2(1+2\delta/\omega),\omega+2\delta} =: \hat{C}_+\tilde{\psi}_{\omega+2\delta}(\mu_1, \mu_2)$$

where we used $1/\mathcal{N}_1 = \sqrt{\mu_1/\mu_2\mu_3} = \mu_1/\omega$ and defined the operator $\hat{C}_+$ acting on the dependence of ψ on μ_1 and μ_2. Thus, unlike for the Schwarzschild interior the difference equation does not become higher order in ω, and the highest order term does have a difference operator coefficient in the remaining independent variables.

The recurrence proceeds as follows: We have a partial difference equation of the form

$$\hat{C}_+\tilde{\psi}_{\omega+2\delta}(\mu_1, \mu_2) + \hat{C}_0\tilde{\psi}_{\omega}(\mu_1, \mu_2) + \hat{C}_-\tilde{\psi}_{\omega-2\delta}(\mu_1, \mu_2)$$

with difference operators $\hat{C}_\pm$ and $\hat{C}_0$ acting on the dependence on μ_1 and μ_2. In terms of initial data at two slices of ω we can solve recursively for $\hat{C}_0\tilde{\psi}_{\omega}(\mu_1, \mu_2) + \hat{C}_-\tilde{\psi}_{\omega-2\delta}(\mu_1, \mu_2) =: \phi(\mu_1, \mu_2)$ and then, in each ω step, use boundary conditions to solve the ordinary difference equation

$$\hat{C}_+\tilde{\psi}_{\omega+2\delta}(\mu_1, \mu_2) = \phi(\mu_1, \mu_2).$$

Although the operator $\hat{C}_+$ itself is not equidistant, this remaining ordinary difference equation can be transformed to an equidistant one by transforming μ_1 and μ_2 as in Sec. III A (using that ω is constant and fixed for this equation at any recursion step). With $\mu_3(\mu_1, \mu_2, \omega) = \omega^2/\mu_1\mu_2$, we have lattice spacings $\mathcal{N}_1(\mu_1, \mu_2, \omega) = \omega/\mu_1$ and $\mathcal{N}_2(\mu_1, \mu_2, \omega) = \omega/\mu_2$ in terms of ω which are already independent of each other. The two remaining variables μ_1 and μ_2 are thus transformed to equidistant ones by taking their logarithms as encountered before.

Note the resemblance of the new variables, volume and two logarithms as the metric components at constant volume, to Misner variables [40]. This observation may be of interest in comparisons with Wheeler-DeWitt quantizations where Misner variables have often been used, making the Wheeler-DeWitt equation hyperbolic.

IV. APPLICATION: STABILITY OF THE SCHWARZSCHILD INTERIOR

Now that we have several possibilities for the lattice spacings, we consider their effect on the solutions of the Hamiltonian constraint. In particular, these solutions may have undesirable properties reminiscent of numerical instabilities, as it was indeed noticed for the original quantization of the Schwarzschild interior in [29]. Also problems in the presence of a positive cosmological constant, described in the introduction, are of this type. Recall that when one wishes to solve an ordinary differential equation, for example, there are various discrete schemes that ensure errors do not propagate as the number of time steps increases. Here we are in the opposite situation—instead of having the freedom to pick the discrete version of a continuous equation, the discrete equation itself is what is fundamental. Thus, like a badly chosen numerical recipe, some choices of the functions N_τ and N_ϑ in the constraint equation may quickly lead to solutions that are out of control, and increase without bound. To test for this, we will use a von Neumann stability analysis [29] on the possible recursion relations. The essential idea is to treat one of the relation parameters as an evolution parameter, and decompose the rest in terms of orthogonal functions, representing "spatial" modes of the solution. This will give rise to a matrix that defines the evolution of the solution; if the matrix eigenvalues are greater than unity for a particular mode, that mode is unstable. In particular, a relation $\sum_{k=-M}^{M} a_{n+k}\psi_{n+k} = 0$ is equivalent to a vector equation of the form $\vec{v}_n = Q(n)\vec{v}_{n-1}$, where the column vector $\vec{v}_n = (\psi_{n+M}, \psi_{n+M-1}, \cdots, \psi_{n-M+1})^T$. The evolution of an eigenvector $\vec{w}$ of the matrix $Q(n)$ is given by $\vec{w}_n = \lambda_w\vec{w}_{n-1}$. Thus, when the size of the corresponding eigenvalue $|\lambda_w| > 1$, the values in the sequence associated to $\vec{w}$ will grow as well.

With this in mind, we consider the choices of N_x and N_ϑ discussed previously, starting with the case $N_x \propto \sqrt{\tau}$ and $N_\vartheta \propto \sqrt{\mu}$. In the large μ, τ limit for this choice, the coefficients of the Hamiltonian constraint become

$$C_\pm(\mu, \tau) \sim 4\delta\sqrt{\frac{\tau}{\mu}}, \qquad C_0(\mu, \tau) \sim \frac{\delta}{\tau}.$$

In the asymptotic limit, the coefficients of the $\psi_{\mu\pm2\delta/\sqrt{\mu},\tau}$ and $\psi_{\mu,\tau}$ terms go to $C_0(\mu, \tau)\mu$. As we saw in Sec. III B, we can choose a different set of variables in which the step-sizes are constant (up to ordering of the operators). Plugging these asymptotic values into the Hamiltonian constraint, and changing variables to $\tilde{\mu} = \mu^{3/2}$ and $\tilde{\tau} = \tau^{3/2}$ gives

$$4\tilde{\tau}(\psi_{\tilde{\mu}+2\delta,\tilde{\tau}+2\delta} - \psi_{\tilde{\mu}-2\delta,\tilde{\tau}+2\delta} + \psi_{\tilde{\mu}-2\delta,\tilde{\tau}-2\delta} - \psi_{\tilde{\mu}+2\delta,\tilde{\tau}-2\delta}) + \tilde{\mu}(\psi_{\tilde{\mu}+4\delta,\tilde{\tau}} - 2\psi_{\tilde{\mu},\tilde{\tau}} + \psi_{\tilde{\mu}-4\delta,\tilde{\tau}}) = 0.$$

Because all the step-sizes now are constants depending on δ, we define new parameters m, n such that $\tilde{\mu} = 2m\delta$ and $\tilde{\tau} = 2n\delta$. Using m as our evolution parameter and n as the spatial direction, we decompose the sequence as $\psi_{2m\delta,2n\delta} = u_m \exp(in\omega)$. With this new function, the recursion relation is written as

$$2in(u_{n+1} - u_{n-1}) - (m\sin\theta)u_n = 0.$$

This is equivalent to the vector equation

$$\begin{bmatrix} u_{n+1} \\ u_n \end{bmatrix} = \begin{bmatrix} -\frac{im}{2n}\sin\theta & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u_n \\ u_{n-1} \end{bmatrix} = Q(m,n) \begin{bmatrix} u_n \\ u_{n-1} \end{bmatrix}. \tag{29}$$

The eigenvalues of the matrix Q are

$$\lambda_\pm = \frac{-im\sin\theta \pm \sqrt{16n^2 - m^2\sin^2\theta}}{4n}.$$

When the discriminant $16n^2 - m^2\sin^2\theta \geq 0$, then $|\lambda| = 1$, and the solution is stable; however, there are unstable modes when $16n^2 - m^2\sin^2\theta < 0$. The most unstable mode corresponds to the choice $\sin\theta = 1$, giving instabilities in terms of the original variables when $\mu > 2\tau$. In this regime, all solutions behave exponentially rather than oscillating. This region includes parts of the classical solutions for the Schwarzschild interior even for values of μ and τ for which one expects classical behavior to be valid. The presence of instabilities implies, irrespective of the physical inner product, that quantum solutions in those regions cannot be wave packets following the classical trajectory, and the correct classical limit is not guaranteed for this quantization, which is analogous to that introduced in [26,37].

The situation is different when we consider the choices $N_\vartheta \propto \sqrt{|\tau|}$ and $N_x \propto \mu/\sqrt{|\tau|}$, where we will find a lack of instability. There is no choice of variables that allows us to asymptotically approach a constant spacing recursion relation, because of the mixing of the μ and τ variables in the step-size functions. Thus, we will make the assumption that in the large μ, τ limit, the solution does not change much under step-sizes δN_x^{-1} and δN_ϑ^{-1}. To see how this affects the resulting stability of the solutions, we will look at a simpler example first. If we start with the Fibonacci relation $R_\tau \equiv \psi_{\tau+1} - \psi_\tau - \psi_{\tau-1} = 0$, then the two independent solutions are of the form $\psi_\tau = \kappa^\tau$, where κ is either the golden ratio $\phi = (1 + \sqrt{5})/2$ or else $-\phi^{-1}$. Only the latter solution meets the criterion for stability, since $|\phi| > 1$. When we change this relation to

$$\tilde{R}_\tau \equiv \psi_{\tau+1/\tau^n} - \psi_\tau - \psi_{\tau-1/\tau^n} = 0, \tag{30}$$

with $n \neq 1$, the situation changes—only one of the two solutions outlined above will solve the relation asymptotically. In particular, when we examine the error $\tilde{R}_\tau$ we get when we plug κ^τ into the altered relation (30), i.e.,

$$\tilde{R}_\tau = \kappa^\tau(\kappa^{1/\tau^n} - 1 - \kappa^{-1/\tau^n}),$$

the error is proportional to ψ_τ itself. As $\tau \to \infty$, therefore, the error for the $\kappa = \phi$ solution grows without bound, while that of $\kappa = -\phi^{-1}$ goes to zero. Thus, we see in this situation a relation between the stability and the asymptotic behavior of a solution.

Returning to the Schwarzschild relation, in the large μ, τ limit the coefficient functions of the recursion relation are to leading order

$$C_\pm(\mu,\tau) \sim 4\delta, \qquad C_0(\mu,\tau) \sim \frac{\delta}{\mu}.$$

In turn, the relation itself becomes

$$\begin{aligned} 4(&\psi_{\mu+2\delta/\sqrt{\tau},\tau+2\delta\sqrt{\tau}/\mu} - \psi_{\mu-2\delta/\sqrt{\tau},\tau+2\delta\sqrt{\tau}/\mu} \\ &- \psi_{\mu+2\delta/\sqrt{\tau},\tau-2\delta\sqrt{\tau}/\mu} + \psi_{\mu-2\delta/\sqrt{\tau},\tau-2\delta\sqrt{\tau}/\mu}) \\ &+ (\psi_{\mu+4\delta/\sqrt{\tau},\tau} - 2\psi_{\mu,\tau} + \psi_{\mu-4\delta/\sqrt{\tau},\tau}) = 0. \end{aligned}$$

From this point on, we assume that we have a solution to this relation which does not vary greatly when, for example, μ is changed by $\pm 2\delta/\sqrt{\mu}$, and similarly for τ. Both N_x and N_ϑ are constant to first order in shifts $\mu \pm 2\delta N_x^{-1}$ and similarly for τ, in the asymptotic limit. Thus, we assume that $\alpha = 2\delta N_x^{-1}$ and $\beta = 2\delta N_\vartheta^{-1}$ are constants, and use the scalings $\mu = \alpha m$ and $\tau = \beta n$. When this is done, we get an equation similar to the case when $N_x \propto \sqrt{\tau}$ and $N_\vartheta \propto \sqrt{\mu}$, but with constant coefficients; this is the crucial difference that allows stable solutions to the case here. Using the decomposition $\psi_{\alpha m,\beta n} = u_n \exp(im\theta)$, we arrive at the matrix equation

$$\begin{bmatrix} u_{n+1} \\ u_n \end{bmatrix} = \begin{bmatrix} -\frac{i}{2}\sin\theta & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u_n \\ u_{n-1} \end{bmatrix}. \tag{31}$$

The matrix here has eigenvalues λ with $|\lambda| = 1$ for all m, n, so the solution is stable. Using arguments as in the Fibonacci example, the nonequidistant equation of the second scheme is shown to be stable.

V. CONCLUSIONS

Following [9], we explicitly introduced loop quantum cosmological models which take into account the full lattice structure of inhomogeneous states. Such lattices are in general refined by adding new vertices when acting with the Hamiltonian constraint. Thus, also dynamical equations even in homogeneous models should respect this property. Several interesting features arose: One obtains nonequidistant difference equations which, when imposed for functions on the whole real line as in isotropic loop quantum cosmology, are more restrictive than equidistant ones due to the absence of superselected sectors. This leaves the singularity issue unchanged since for this one only needs to consider a few steps in the equation. But a stability analysis of solutions and the verification of the correct classical limit in all semiclassical regimes can be more challenging. We presented an example for such an analysis, but also introduced a procedure by which one can transform the resulting equations to equidistant ones up to quantum corrections, which is sufficient for a semiclassical analysis. Interestingly, properties of the transformation itself provide hints to the correct semiclassical behavior.

As a side-result, we demonstrated that one particular version of lattice refinements naturally gives rise to Misner-type variables.

It is our understanding that this general procedure of defining lattice refining models mostly agrees with the intuition used specifically in isotropic models in [26], and adapted to anisotropic ones in [37,41]. However, there are some departures from what is assumed in [26]. First, we do not see indications to refer to the area operator while the area spectrum was not only used in [26] to fix the constant δ and the volume dependence of the step-size but in fact provided the main motivation. Second, due to this motivation [26] presents a more narrow focus which from our viewpoint corresponds to only one single refinement model. It has a vertex number proportional to volume, which is a limiting case not realized by known full Hamiltonian constraints, and puts special emphasis on geometrical areas to determine the vertex number. Finally, commutators for inverse volume operators are to be treated differently from [26], taking into account a lattice refining model which would not be possible in a purely homogeneous formulation. As shown in the Appendix, this enlarges expected quantum corrections to the classical functions.

We have discussed similar cases for illustration here, but keep a more general viewpoint on the refinement as a function of volume. A preliminary stability analysis for the Schwarzschild interior, consistent with [42] indeed suggests that a behavior different from what is suggested in [26] is preferred, which indicates that models can provide tight conditions for the general analysis of quantum dynamics. We emphasize that stability arguments as used here are independent of physical inner product issues since they refer to properties of *general solutions*. A general analysis as started here allows detailed tests of the full dynamics in manageable settings, which can verify the self-consistency of the framework of loop quantum gravity—or possibly point to limitations which need to be better understood.

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APPENDIX A: INVERSE VOLUME TERMS IN HOMOGENEOUS MODELS AND LATTICE REFINEMENT

We have seen in this paper, following [9], that Hamiltonian constraint operators with triad-dependent parameters in holonomies allow one to model lattice refinements faithfully, with interesting results and some improvements over the original nonrefining models. However, as always there are also some features of inhomogeneous states and operators which are not present and difficult to mimic in homogeneous models. Thus, even models generalized in this way by allowing for lattice refinement effects have to be interpreted with great care. While qualitative effects can be investigated fruitfully to test the full framework, there is no basis for drawing quantitative conclusions. The prime example is that of commutator terms which appear ubiquitously in composite operators of loop quantum gravity, such as the coefficients of difference equations or also matter Hamiltonians.

In the main construction of this paper we used holonomies associated with links of a lattice, rather than edges of a fixed coordinate length. This allows us, effectively, to take into account lattice refinements which change the number of vertices. It applies to holonomies (16) along a closed loop used to quantize curvature components which determine the step-size of difference equations, but also to the link holonomies used in commutators to quantize inverse triad components based on (14). What is not modeled in homogeneous models is the fact that a lattice operator makes use of the *local* volume $\hat{V}_v$ at a given vertex v where the commutator is acting, rather than the *total* volume $\hat{V} = \sum_v \hat{V}_v$ of the whole box in which the lattice is embedded. In a fully inhomogeneous setting the difference does not matter since volume contributions from vertices not touched by the edge used in a commutator drop out in the end, $[h_e, \hat{V}] = \sum_{v\in e}[h_e, \hat{V}_v]$. But in homogeneous models there is a difference since volume contributions from different vertices, in an exactly homogeneous setting, are all identical. Thus, the total volume $V = \mathcal{N}V_v$ is the number of vertices multiplied with the local volume V_v. Then, $[h, \hat{V}_v]$ rather than $[h, \hat{V}]$ is expected as the contribution to constraint operators from the inhomogeneous perspective. In homogeneous models as in [26], on the other hand, $[h, \hat{V}]$ is more straightforward to use. We now show that without corrections this would imply crucial deviations from the inhomogeneous behavior.

It is easy to see that commutators differ depending on whether the local or total volume is used. For simplicity of the argument, we proceed with an isotropic situation where $V = |p|^{3/2}$ in terms of the basic isotropic densitized triad component p. A local lattice flux, for a surface S intersecting only a single link, would be $\rho = \int_S \mathrm{d}^2y\tilde{p} = \ell_0^2 p/L_0^2 = p/\mathcal{N}^{2/3}$ for links of coordinate length ℓ_0, such that $V_v = |\rho|^{3/2} = |p|^{3/2}/\mathcal{N}$ is the local volume. (We again use a coordinate box of size L_0^2 and introduce rescaled flux variables $p = L_0^2\tilde{p}$.) Isotropic states are spanned by $e^{i\mu c/2}$ where $\mu \in \mathbb{R}$ is related to the triad eigenvalues by $p_\mu = 4\pi\gamma\ell_{\mathrm{P}}^2\mu/3$. Using a link holonomy $h \sim e^{i\ell_0\tilde{c}/2} = e^{ic/2\mathcal{N}^{1/3}}$ which as a multiplication operator increases μ by $1/\mathcal{N}^{1/3}$, a commutator with the total volume will have

eigenvalues of the form

$$h^{-1}[h,\hat{V}] \sim V(\mu+1/\mathcal{N}^{1/3}) - V(\mu-1/\mathcal{N}^{1/3}) = |p+4\pi\gamma\ell_{\mathrm{P}}^2/3\mathcal{N}^{1/3}|^{3/2} - |p-4\pi\gamma\ell_{\mathrm{P}}^2/3\mathcal{N}^{1/3}|^{3/2}. \tag{A1}$$

If the local volume is used, on the other hand, we have to refer to local edge labels $\mu_e = 3\rho/4\pi\gamma\ell_{\mathrm{P}}^2$, rather than using the total p. Thus,

$$\begin{aligned} h_e^{-1}[h_e,\hat{V}_v] &\sim V_v(\mu_e+1) - V_v(\mu_e-1) \\ &= |\rho+4\pi\gamma\ell_{\mathrm{P}}^2/3|^{3/2} - |\rho-4\pi\gamma\ell_{\mathrm{P}}^2/3|^{3/2} \\ &= \mathcal{N}^{-1}(|p+4\pi\gamma\ell_{\mathrm{P}}^2\mathcal{N}^{2/3}/3|^{3/2} \\ &\quad - |p-4\pi\gamma\ell_{\mathrm{P}}^2\mathcal{N}^{2/3}/3|^{3/2}). \end{aligned} \tag{A2}$$

For large volume, $p \gg \mathcal{N}$, both expressions give the correct classical limit $\frac{3}{2}\mathcal{N}^{-1/3}\sqrt{|p|}$ expected from $\{e^{ic/2N^{1/3}}, |p|^{3/2}\}$. However, quantum corrections, i.e., deviations from this classical limit for finite p, are much larger for the second version using the local volume as it would occur in an inhomogeneous quantization. The smooth classical function $\mathrm{d}V/\mathrm{d}p$ in a Poisson bracket appears in discretized form by the large step-size $N^{2/3}$ in (A2) rather than the small one $N^{-1/3}$ in (A1). Perturbative corrections, derived by Taylor expanding the difference terms and keeping higher order corrections to the classical expression, are thus larger. (This can have cosmological implications [43–45].) Nonperturbative effects as observed for the inverse scale factor operator in isotropic loop quantum cosmology which has an upper bound at finite volume [46], start to arise for $p \sim \mathcal{N}^{2/3}$ when the local volume is used but only at the much smaller $p \sim \mathcal{N}^{-1/3}$ for the total volume. Since only the local volume is relevant for inhomogeneous quantizations, quantum corrections from inverse volume operators can be large.

Unfortunately, this effect is more difficult to mimic in exact homogeneous models unlike the behavior of holonomies under lattice refinements and has therefore been overlooked in [26]. The connection components appearing in holonomies can simply be divided by a function $\mathcal{N}$ of triad components to implement shrinking edges due to subdivision. For the volume itself it is not possible to use a local version in a homogeneous model since, if we would divide the total volume by the appropriate function of triad components, only a constant would remain for an $\mathcal{N}$ proportional to volume and the commutator would be zero. The only way to have this effect faithfully implemented in a homogeneous model is to use higher SU(2) representations for holonomies in commutators but *not* for holonomies used in the loop to quantize curvature components. (This is not possible if one writes the constraint as a single trace, $\mathrm{tr}(h_\alpha h_e[h_e^{-1},\hat{V}])$, but can easily be done using the equivalent form $\mathrm{tr}(\tau_i h_\alpha)\,\mathrm{tr}(\tau_i h_e[h_e^{-1},\hat{V}])$. We emphasize that higher representations for commutators are advocated here only in exactly homogeneous models to mimic inhomogeneous effects. Fully inhomogeneous operators usually need not refer to higher representations.) In a representation of spin j, matrix elements of holonomies contain exponentials $\exp(imc/2\mathcal{N}^{1/3})$ with $-j \le m \le j$, which increases the shifts in volume labels resulting from commutators. Resulting expressions for commutators can be found in [47,48]. If the representation label j is of the order $\mathcal{N}$, effects as they result from lattice refinements and using the local volume are correctly implemented. Accordingly, corrections from inverse triad components quantized through commutators are much larger than they would otherwise be [49].

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does not present a true Hamiltonian. Refinement, as we use it, happens with respect to an internal time variable such as the volume. The lattice behavior is then more indirectly related to the action of the fundamental Hamiltonian, which makes a specific determination of the refinement complicated. Nevertheless, with respect to volume as internal time refinements of a lattice dominate over coarsenings because the creation of new vertices usually increases the volume while removing a vertex would decrease the volume. Even for a self-adjoint Hamiltonian constraint operator the balance between the creation and removal of vertices and edges is broken in the refinement picture as a consequence of using the volume as internal time with respect to which refinements are described. (See also the discussion in [51]).

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