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Diffeomorphism Covariance and the Quantum Schwarzschild Interior

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Abstract: We introduce a notion of residual diffeomorphism covariance in quantum Kantowski–Sachs (KS) describing the interior of a Schwarzschild black hole. We solve for the family of Hamiltonian constraint operators satisfying the associated covariance condition, as well as parity invariance, preservation of the Bohr Hilbert space of the Loop Quantum KS and a correct (naïve) classical limit. We further explore the imposition of minimality for the number of terms and compare the solution with those of other Hamiltonian constraints proposed for the Loop Quantum KS in the literature. In particular, we discuss a lapse that was recently commonly chosen due to the resulting decoupling of the evolution of the two degrees of freedom and the exact solubility of the model. We show that such a choice of lapse can indeed be quantized as an operator that is densely defined on the Bohr Hilbert space and that any such operator must include an infinite number of shift operators.

Keywords: quantum gravity; diffeomorphisms; black holes

Citation: Bornhoeft, I.W.; Dias, R.G.; Engle, J.S. Diffeomorphism Covariance and the Quantum Schwarzschild Interior. *Universe* **2024**, *10*, 89. https://doi.org/10.3390/universe10020089

Academic Editor: Parampreet Singh

Received: 13 January 2024
Revised: 8 February 2024
Accepted: 11 February 2024
Published: 13 February 2024

1. Introduction

A central epistemic value in science is that of simplicity —that a theory be derived uniquely from as few principles as possible. It follows that it is important to eliminate, as much as possible, ambiguities that are present in a theory through physical principles, particularly when observational data are scarce.

General relativity is based on background independence, which is equivalent to covariance under diffeomorphisms [1]. Guided by this principle, loop quantum gravity (LQG) is a non-perturbative approach to a quantum theory of gravity [1–6], and loop quantum cosmology (LQC) models arise from applying quantization techniques analogous to LQG to symmetry-reduced gravitational models [7–9]. In order to ensure that a given LQC model faithfully reflects the diffeomorphism covariance of full loop quantum gravity, it is important for this model to also be diffeomorphism-covariant in some sense, a requirement that can also serve to reduce ambiguities in its construction. Related prior work along these lines includes the following:

- Lewandowski, Okolow, Sahlmann, and Thiemann [10] proved that the requirement of invariance under spatial diffeomorphisms—or, more precisely, the unitary implementation of the action of the diffeomorphism group—establishes the uniqueness of the kinematics of LQG.
- For LQC, Ashtekar and Campiglia [11] showed that, in the case of the Bianchi I model, a unique kinematical representation is achieved through invariance under canonical and, thus, volume-preserving residual diffeomorphisms, i.e., diffeomorphisms that are not frozen by the gauge fixing required by symmetry reduction.
- The works [12,13] extended the result to single out the standard kinematical Hilbert space of the homogeneous isotropic case by also requiring invariance under non-canonical residual diffeomorphisms.

- The works [14,15] demonstrated, for the cases of homogeneous isotropic LQC and Bianchi I models, that a family of dynamics can also be derived from residual diffeomorphism covariance, and, if desired, uniqueness can be achieved by requiring minimality—a form of Occam's razor requiring the Hamiltonian to have a minimal number of terms, i.e., a minimal number of shift operators—in addition to a further assumption of planar loops for the Bianchi I case.

In this work, we investigate the choice of dynamics for the loop quantization of the Schwarzschild black hole interior described by the Kantowski–Sachs (KS) framework. There is a wide literature discussing different proposals for such a choice (for instance, [16–26]). Here, instead of quantizing the Hamiltonian directly, we narrow the possibilities by imposing physically motivated properties, namely, the following:

- Covariance under residual diffeomorphisms. Looking at how the phase-space variables flow under the action of the residual diffeomorphisms (Section 3), we formulate a condition for the covariance of the Hamiltonian, which we quantize, establishing a condition of quantum covariance under such diffeomorphisms. The residual diffeomorphisms are non-canonical, so this requires novel methods (Section 4).
- Covariance under discrete residual automorphisms of the $SU(2)$ principal fiber bundle (Section 5).
- The correct (naïve) classical limit (Section 6).

In addition to these basic physical criteria, we also consider the consequences of the additional criterion of minimality—that the quantum Hamiltonian constraint contains a minimal number of shift operators (Section 7).

The naïve classical limit, which has been used in all of the LQC and loop quantum KS literature up until now, corresponds to $\hbar \to 0$, the limit in which the Planck length $\ell_P := \sqrt{G\hbar}$ goes to zero, or, equivalently, the limit under which the length of curves regularizing curvature and connection factors in the Hamiltonian constraint goes to zero; in Section 6.1, we show that this is equivalent to the eigenvalues of extrinsic curvature going to zero. This is the definition of classical limit used in this paper, as the focus of this study is not to develop a new one. However, this definition of classical limit is limited because the truly relevant criterion for the classical regime is that four-dimensional curvature scalars should go to zero, which can happen even if the eigenvalues of extrinsic curvature do not. Indeed, in KS, this happens at the horizon, where the latter diverge, while the former remain small compared to the Planck scale. This is, in fact, the regime in which the model of Ashtekar, Olmedo, and Singh (AOS) [23,26], as well as the earlier models [21,27], perform better than all other models, and this is remarked upon in Section 8.3.

In Section 6.3, we present a discussion of a choice of lapse used in the literature that greatly simplifies the classical and (with further assumptions) effective equations, rendering them analytically solvable. In particular, we prove that the quantum Hamiltonian operator resulting from such a choice can be densely defined on the usual Bohr Hilbert space motivated by loop quantum gravity only with an infinite number of shift operators.

For completeness—and to fix the notation—we start with a background review of the KS framework and its loop quantum kinematics (Section 2). To finish, we compare our conclusions with other proposals in the literature (Section 8).

2. Background

2.1. Kantowski–Sachs in Ashtekar–Barbero Variables

The interior region of a Schwarzschild black hole can be foliated in homogeneous 3-manifolds of topology $\mathbb{R} \times S^2$, which are invariant under the Kantowski–Sachs group $\mathbb{R} \times SO(3)$. We introduce standard coordinates (θ, ϕ) on the S^2 factor and a coordinate x on the $\mathbb{R}$ factor, as well as a fiducial cell of coordinate length L_o in the non-compact x direction as an infrared cutoff, to prevent integrations from diverging. The physical results are required to be independent of this parameter.

The geometry is characterized by a symmetry-reduced phase space described by two conjugate pairs of variables (b, p_b) and (c, p_c), with Poisson brackets

$$\{b, p_b\} = G\gamma \quad , \quad \{c, p_c\} = 2G\gamma. \tag{1}$$

In terms of these, the Ashtekar–Barbero connection and densitized triad are given by

$$\begin{aligned} A_a^1 &= -b\sin\theta\partial_a\phi \quad , \quad E_1^a = -\frac{p_b}{L_0}\phi^a, \\ A_a^2 &= b\partial_a\theta \quad , \quad E_2^a = \frac{p_b}{L_0}\sin\theta\theta^a, \\ A_a^3 &= \frac{c}{L_0}\partial_a x + \cos\theta\partial_a\phi \quad , \quad E_3^a = p_c\sin\theta x^a \end{aligned} \tag{2}$$

where ϕ^a, θ^a, and x^a denote the coordinate vector fields. The corresponding homogeneous spacetime metric is given by

$$ds^2 = -N^2 d\tau^2 + \frac{p_b^2}{|p_c|L_0^2}dx^2 + |p_c|d\Omega^2, \tag{3}$$

which can be identified with the Schwarzschild interior metric

$$ds^2 = -\left(\frac{2m}{\tau} - 1\right)^{-1} d\tau^2 + \left(\frac{2m}{\tau} - 1\right)dx^2 + \tau^2 d\Omega^2,$$

for $\tau < 2m$ by choosing the lapse and consequent evolution of the momenta to be

$$|p_c| = \tau^2, \qquad p_b^2 = L_0^2\left(\frac{2m}{\tau} - 1\right)\tau^2, \qquad N^2 = \left(\frac{2m}{\tau} - 1\right)^{-1}. \tag{4}$$

Returning now to the case of the general lapse, from Equation (2), one can calculate the Hamiltonian constraint to be

$$H_{c\ell}[N] = -\frac{N}{2G\gamma^2}\frac{b\,\mathrm{sgn}\,p_c}{\sqrt{|p_c|}}\left(p_b\left(b + \frac{\gamma^2}{b}\right) + 2cp_c\right), \tag{5}$$

for an arbitrary lapse N. Letting $V = 4\pi|p_b|\sqrt{|p_c|}$ denote the physical volume of the fiducial cell, we choose a family of lapses of the form

$$N = V^n = \left(4\pi|p_b|\sqrt{|p_c|}\right)^n, \tag{6}$$

for $n > -3$. This covers the cases of proper time ($n = 0$, as in [17,20]) and the harmonic time gauge ($n = 1$, as in [19]), among others—for instance, the case $n = -1$ appears when considering unimodular gravity [25]. From now on, we will assume this choice of lapse and simply represent $H_{c\ell}[N]$ as $H_{c\ell}$. There is a choice of lapse prominent in the literature that does not fall into this family; we discuss this choice in Section 6.3. The restriction $n > -3$ will be needed in Section 4.2. The classical Hamiltonian constraint (5) then becomes

$$\begin{aligned} H_{c\ell} &= -\frac{(4\pi)^n|p_b|^n|p_c|^{\frac{(n-1)}{2}}b\,\mathrm{sgn}\,p_c}{2G\gamma^2}\left(p_b\left(b + \frac{\gamma^2}{b}\right) + 2cp_c\right) \\ &= -\frac{V^{n+1}}{8\pi G\gamma^2}\,\mathrm{sgn}\,p_b\left(\frac{b^2+\gamma^2}{p_c} + \frac{2bc}{p_b}\right). \end{aligned} \tag{7}$$

2.2. Quantum Kinematics

The basic configuration variables with direct quantum analogs in loop quantum gravity and loop quantizations of symmetry-reduced models are always some class of holonomies $h_e[A]$. For the Kantowski–Sachs framework, one considers holonomies along curves parallel to the x axis along x = constant curves that are geodesic with respect to the two-sphere metric:

$$\begin{aligned} h_x[A] &= \exp\left(-i\frac{\lambda c}{2}\sigma_3\right) = \cos\left(\frac{\lambda c}{2}\right)\mathbb{I} - i\sin\left(\frac{\lambda c}{2}\right)\sigma_3 \\ h_\theta[A] &= \exp\left(-i\frac{\mu b}{2}\sigma_2\right) = \cos\left(\frac{\mu b}{2}\right)\mathbb{I} - i\sin\left(\frac{\mu b}{2}\right)\sigma_2 \\ h_\phi[A]|_{\theta=\frac{\pi}{2}} &= \exp\left(i\frac{\mu b}{2}\sigma_1\right) = \cos\left(\frac{\mu b}{2}\right)\mathbb{I} + i\sin\left(\frac{\mu b}{2}\right)\sigma_1. \end{aligned} \tag{8}$$

where σ_i are the Pauli matrices. The matrix elements of these holonomies generate the algebra of almost-periodic functions, which are composed of elements of the form

$$f(b,c) = \sum_{j=1}^{N} f_j e^{\frac{i}{2}(\mu_j b + \lambda_j c)}, \tag{9}$$

where N is possibly infinite, $f_j \in \mathbb{C}$, and $\mu_j, \lambda_j \in \mathbb{R}$. The space of such functions endowed with—and normalizable with respect to—the inner product

$$\left\langle e^{\frac{i}{2}(\mu_j b + \lambda_j c)} \middle| e^{\frac{i}{2}(\mu_k b + \lambda_k c)} \right\rangle := \lim_{L\to\infty} \frac{1}{(2L)^2} \int_{(-L,L)^2} \overline{e^{\frac{i}{2}(\mu_j b + \lambda_j c)}} e^{\frac{i}{2}(\mu_k b + \lambda_k c)} \mathrm{d}b\mathrm{d}c = \delta^{\mu_k}_{\mu_j} \delta^{\lambda_k}_{\lambda_j},$$

is called the Bohr Hilbert space, which is denoted by $\mathcal{H}_{\mathrm{Bohr}}$ and is the space of kinematical states for the quantum theory. The momenta are quantized as

$$\hat{p}_b = -i\gamma\ell_P^2 \frac{\partial}{\partial b}, \qquad \hat{p}_c = -2i\gamma\ell_P^2 \frac{\partial}{\partial c}, \tag{10}$$

so that each associated normalized simultaneous eigenstate $|p_b, p_c\rangle$ has the wavefunction $\psi_{p_b,p_c}(b,c) = e^{\frac{i}{\gamma\ell_P^2}\left(p_b b + \frac{p_c c}{2}\right)}$. Equation (9) can then also be written as

$$f(b,c) = \sum_{j=1}^{N} f_j |p_b^j, p_c^j\rangle. \tag{11}$$

Complex exponentials of b and c then act as shift operators:

$$e^{i\eta b}|p_b^j, p_c^j\rangle = |p_b^j + \gamma\ell_P^2\eta, p_c^j\rangle \qquad \text{and} \qquad e^{i\eta c}|p_b^j, p_c^j\rangle = |p_b^j, p_c^j + 2\gamma\ell_P^2\eta\rangle.$$

3. Residual Diffeomorphisms

The kinematical symmetry group of the Ashtekar–Barbero formulation of gravity is the group Aut of automorphisms of the $SU(2)$ principle bundle, which is isomorphic to the semi-direct product of diffeomorphisms of the spatial slice and $SU(2)$ gauge rotations. The subgroup $\overline{\mathrm{Aut}}$ of Aut preserving the form (2) of the phase-space variables (A_a^i, E_i^a) yields a well-defined action on the parameters (b, c, p_b, p_c) via

$$\varphi \triangleright \Big((A_a^i, E_i^a)(b, c, p_b, p_c) \Big) =: (A_a^i, E_i^a)(\varphi \triangleright (b, c, p_b, p_c)) \tag{12}$$

for all $\varphi \in \overline{\mathrm{Aut}}$. We call the quotient Aut_R of $\overline{\mathrm{Aut}}$ from the kernel of this action the group of residual automorphisms in the KS framework. The identity component of Aut_R consists of spatial diffeomorphisms; we refer to it as the group of residual diffeomorphisms for KS and denote it by Diff_R. If we let $\overline{\mathrm{Diff}}$ denote the subgroup of $\overline{\mathrm{Aut}}$ consisting of spatial diffeomorphisms, then Diff_R can also be calculated as the quotient of $\overline{\mathrm{Diff}}$ from the kernel of its action in Equation (12). In the present section, we solve for the group

Diff_R. The remaining discrete elements of Aut_R, which consist of the parity maps and their compositions, will be discussed in Section 5.

To solve for Diff_R, we first solve for $\overline{\mathrm{Diff}}$ by finding the most general one-parameter family of diffeomorphisms $s \mapsto \Phi^s_{\vec{v}}$, which are generated by some smooth vector field $\vec{v}$ and preserve the form of (2), so that

$$\Phi^s_{\vec{v}} \triangleright \Big((A^i_a, E^a_i)(b, c, p_b, p_c) \Big) =: (A^i_a, E^a_i)(b(s), c(s), p_b(s), p_c(s)) \tag{13}$$

for some set of functions $(b(s), c(s), p_b(s), p_c(s))$. Taking the derivative of both sides with respect to s yields

$$\begin{aligned} \mathcal{L}_{\vec{v}} A^i_a(s) &= \dot{A}^i_a = \frac{\partial A^i_a}{\partial b}\dot{b}(s) + \frac{\partial A^i_a}{\partial c}\dot{c}(s), \\ \mathcal{L}_{\vec{v}} E^a_i(s) &= \dot{E}^a_i = \frac{\partial E^a_i}{\partial p_b}\dot{p}_b(s) + \frac{\partial E^a_i}{\partial p_c}\dot{p}_c(s). \end{aligned} \tag{14}$$

Note that $\dot{b}, \dot{c}, \dot{p}_b, \dot{p}_c$, like b, c, p_b, p_c, are constant in space. The set of all $\vec{v}$ satisfying these relations for some $\dot{b}$, $\dot{c}$, $\dot{p}_b$, and $\dot{p}_c$ will then generate $\overline{\mathrm{Diff}}$. We proceed to derive the consequences of each of these conditions in the most convenient order:

- A^2_a:

  $$\mathcal{L}_{\vec{v}} A^2_a = v^b \partial_b (b \partial_a \theta) + b \partial_b \theta \partial_a v^b = b \left(\frac{\partial v^\theta}{\partial x}\partial_a x + \frac{\partial v^\theta}{\partial \theta}\partial_a \theta + \frac{\partial v^\theta}{\partial \phi}\partial_a \phi \right),$$

  which must be equal to $\dot{A}^2_a = \dot{b}\partial_a\theta$, yielding

  $$\frac{\partial v^\theta}{\partial x} = \frac{\partial v^\theta}{\partial \phi} = 0 \quad \text{and} \quad \dot{b}(s) = b\frac{\partial v^\theta}{\partial \theta}.$$

  Since b and $\dot{b}$ are constant in space, so is $\frac{\partial v^\theta}{\partial \theta}$, which, together with the first two equations above, implies $v^\theta = \kappa_\theta \theta + \xi_\theta$ for some $\kappa_\theta, \xi_\theta \in \mathbb{R}$. However, the smoothness of $\vec{v}$ requires that $v^\theta = 0$ at $\theta = 0$ and $\theta = \pi$, forcing $\kappa_\theta = \xi_\theta = 0$, whence

  $$v^\theta \equiv 0 \tag{15}$$

  and

  $$\mathcal{L}_{\vec{v}} A^2_a = 0. \tag{16}$$

- A^1_a:

  $$\begin{aligned} \mathcal{L}_{\vec{v}} A^1_a &= v^b \partial_b(-b \sin\theta \partial_a \phi) - b \sin\theta (\partial_b \phi)\partial_a v^b \\ &= -b v^b \cos\theta \partial_b \theta \partial_a \phi - b \sin\theta \partial_a v^\phi \\ &= -b\left(\cos\theta v^\theta + \sin\theta \frac{\partial v^\phi}{\partial \phi} \right)\partial_a \phi - b\sin\theta \frac{\partial v^\phi}{\partial \theta}\partial_a\theta - b\sin\theta\frac{\partial v^\phi}{\partial x}\partial_a x, \end{aligned}$$

  which, by Equation (14), must be equal to $\dot{A}^1_a = -\dot{b}(s)\sin\theta\partial_a\phi$. This, with Equation (15), implies

  $$\frac{\partial v^\phi}{\partial \theta} = \frac{\partial v^\phi}{\partial x} = 0 \quad \text{and} \quad \dot{b}(s) = b\frac{\partial v^\phi}{\partial \phi}.$$

Thus, by the same argument used for v^θ, we conclude that $v^\phi = \kappa_\phi \phi + \xi_\phi$ for some constants $\kappa_\phi, \xi_\phi \in \mathbb{R}$. The smoothness of $\vec{v}$ now requires $v^\phi(\phi = 0) = v^\phi(\phi = 2\pi)$, forcing $\kappa_\phi = 0$, so that

$$v^\phi = \text{constant} =: \xi_\phi \tag{17}$$

and

$$\mathcal{L}_{\vec{v}} A^1_a = 0. \tag{18}$$

- A^3_a:

$$\begin{aligned}\mathcal{L}_{\vec{v}} A^3_a &= v^b \partial_b \left(\frac{c}{L_0} \partial_a x + \cos\theta \partial_a \phi \right) + \left(\frac{c}{L_0} \partial_b x + \cos\theta \partial_b \phi \right) \partial_a v^b \\ &= -\sin\theta v^\theta \partial_a \phi + \frac{c}{L_0} \partial_a v^x + \cos\theta \phi \partial_a v^\phi \\ &= \frac{c}{L_0} \frac{\partial v^x}{\partial \phi} \partial_a \phi + \frac{c}{L_0} \frac{\partial v^x}{\partial \theta} \partial_a \theta + \frac{c}{L_0} \frac{\partial v^x}{\partial x} \partial_a x\end{aligned}$$

where, in going from the second to the third line, we used Equations (15) and (17). Requiring this to be equal to $\dot{A}^3_a = \frac{\dot{c}}{L_0} \partial_a x$ then implies

$$\frac{\partial v^x}{\partial \phi} = \frac{\partial v^x}{\partial \theta} = 0 \qquad \text{and} \qquad \dot{c} = c \frac{\partial v^x}{\partial x}.$$

Since c and $\dot{c}$ are constant in space, the same argument as that used for v^θ and v^ϕ again applies here, so

$$v^x = \kappa_x x + \xi_x \tag{19}$$

for some constants $\kappa_x, \xi_x \in \mathbb{R}$—this time unconstrained by the smoothness of $\vec{v}$—and

$$\mathcal{L}_{\vec{v}} A^3_a = \frac{\kappa_x c}{L_0} \partial_a x. \tag{20}$$

The restrictions (15) to (19) thereby fix

$$\vec{v} = \xi_\phi \vec{\phi} + (\xi_x + \kappa_x x) \vec{x}, \tag{21}$$

where $\xi_\phi, \xi_x, \kappa_x$ are free constant parameters. One can check that the remaining conditions in Equation (14) are automatically satisfied with no further restrictions on $\vec{v}$—explicitly, from $\mathcal{L}_v E^a_i = v^c \partial_c E^a_i - E^c_i \partial_c v^a + E^a_i \partial_c v^c$,

$$\mathcal{L}_v E^a_1 = -\frac{\kappa_x p_b}{L_0} \phi^a, \tag{22}$$

$$\mathcal{L}_v E^a_2 = \frac{\kappa_x p_b}{L_0} \sin\theta \theta^a, \tag{23}$$

$$\mathcal{L}_v E^a_3 = 0. \tag{24}$$

Therefore, $\{\vec{\phi}, \vec{x}, x\vec{x}\}$ is a basis of the vector fields generating $\overline{\text{Diff}}$. Note that the resulting flows—Equations (16), (18), (20), and (22)–(24)—depend only on κ_x and not on ξ_x or ξ_ϕ. The reason is easily found to be from the significance of the corresponding vector fields:

- $\vec{\phi}$ generates part of the spherical symmetry manifest in Schwarzschild. The other two spatial rotations are not manifest here as symmetries because we are looking at symmetries of (A^i_a, E^a_i)—full spherical symmetry can be imposed on (A^i_a, E^a_i) at most up to $SU(2)$ gauge rotations and is manifest only in $SU(2)$-gauge-invariant structures constructed from them, such as the 3-metric (3).

- $\vec{x}$ generates translations in x, which corresponds to t in the usual form of the Schwarzschild solution, so this symmetry corresponds to the t-translation symmetry in Schwarzschild.
- $x\vec{x}$ generates something more interesting: An exponential flow in the x direction, and the only flow with non-trivial action on (A_a^i, E_i^a).

Thus, the kernel K of the action of $\overline{\text{Diff}}$ on (A_a^i, E_i^a) is generated by $\vec{\phi}$ and $\vec{x}$, so the group of residual diffeomorphisms $\text{Diff}_R := \overline{\text{Diff}}/K$ is one-dimensional and parameterized by κ_x. Rescaling $\vec{v}$ in Equation (21) is equivalent to rescaling the parameter time s for the flow generated so that we can, without loss of generality, take $\kappa_x = 1$. With this choice, the resulting flow of the phase-space variables (b, p_b, c, p_c) is given by

$$\dot{b} = 0, \qquad \dot{p}_b = p_b, \qquad \dot{c} = c, \qquad \dot{p}_c = 0. \tag{25}$$

The volume of the fiducial cell then flows as $\dot{V} = 4\pi|\dot{p_b}|\sqrt{|p_c|} = 4\pi|p_b|\sqrt{|p_c|} = V$, and, hence, the flow of the Hamiltonian constraint is of the form

$$\dot{H}_{c\ell} = (n+1)H_{c\ell}. \tag{26}$$

4. Covariance Equation

4.1. Strategy

Classically, the flow of a phase-space function F under a family of canonical transformations generated by phase-space function Λ is given by

$$\dot{F} = \{\Lambda, F\}. \tag{27}$$

The standard quantization procedure then turns functions into operators and Poisson brackets into commutators, yielding the following evolution with respect to the flow parameter s:

$$\dot{F} = \frac{1}{i\hbar}[\hat{\Lambda}, \hat{F}] \qquad \Rightarrow \qquad \hat{F}(s) = e^{\frac{s}{i\hbar}\hat{\Lambda}}\hat{F}(0)e^{-\frac{s}{i\hbar}\hat{\Lambda}}.$$

The residual diffeomorphism flow in Kantowski–Sachs, however, does not preserve Poisson brackets and, thus, is non-canonical. As we shall now prove, however, the flow can be cast in a form related to Equation (27),

$$\dot{F} = \omega_1(b, p_b)\{\Lambda_1(b, p_b), F\} + \omega_2(c, p_c)\{\Lambda_2(c, p_c), F\}. \tag{28}$$

Substituting this form into Equation (25) for the residual diffeomorphisms' flow yields

$$0 = -\gamma G\omega_1\frac{\partial\Lambda_1}{\partial p_b}, \quad p_b = \gamma G\omega_1\frac{\partial\Lambda_1}{\partial b}, \quad c = -2\gamma G\omega_2\frac{\partial\Lambda_2}{\partial p_c}, \quad 0 = 2\gamma G\omega_2\frac{\partial\Lambda_2}{\partial c}.$$

The first and last equations tell us that $\Lambda_1 = \Lambda_1(b)$ and $\Lambda_2 = \Lambda_2(p_c)$ are each a function of only one variable. The remaining equations then determine ω_1 and ω_2 in terms of Λ_1 and Λ_2,

$$\omega_1(b, p_b) = \frac{p_b}{\gamma G\frac{\partial\Lambda_1(b)}{\partial b}}, \qquad \omega_2(c, p_c) = -\frac{c}{2\gamma G\frac{\partial\Lambda_2(p_c)}{\partial p_c}}.$$

Therefore, the only free parameters are $\Lambda_1(b)$ and $\Lambda_2(p_c)$, with a restriction that their first derivatives do not vanish, except possibly on a set of measure zero. Arguably, the simplest choice is to make $\Lambda_1(b)$ and $\Lambda_2(p_c)$ proportional to b and p_c, respectively. The choice of proportionality constant does not affect the final quantum covariance condition, so, without loss of generality, we set

$$\Lambda_1 = b \quad \Rightarrow \quad \omega_1 = \frac{p_b}{\gamma G}.$$
$$\Lambda_2 = p_c \quad \Rightarrow \quad \omega_2 = -\frac{c}{2\gamma G}. \tag{29}$$

With this choice, Equation (26) takes the form

$$\dot{H}_{c\ell} = \frac{p_b}{\gamma G}\{b, H_{c\ell}\} - \frac{c}{2\gamma G}\{p_c, H_{c\ell}\} = (n+1)H_{c\ell}. \tag{30}$$

It is Equation (30) that we will quantize to obtain a quantum covariance condition on the constraint operator $\hat{H}$. Since b and c appear directly in this equation without exponentiation and since $\hat{b}$ and $\hat{c}$ are not well defined on the Bohr Hilbert space arising from loop quantization (as reviewed in Section 2.2), we first find the general solution to this equation in the standard Schrödinger representation, with a subsequent imposition of preservation of the Bohr Hilbert space.

4.2. Quantization in the Schrödinger Representation and General Solution for the Matrix Elements

We follow the standard quantization procedure, choosing the Weyl ordering for quantizing products, $\hat{A} \star \hat{B} := \frac{1}{2}(\hat{A}\hat{B} + \hat{B}\hat{A})$, yielding

$$\begin{aligned}(n+1)\hat{H} &= \frac{1}{i\hbar}\left(\hat{\omega}_1 \star [\hat{\Lambda}_1, \hat{H}] + \hat{\omega}_2 \star [\hat{\Lambda}_2, \hat{H}]\right) \\ &= \frac{1}{2i\gamma\ell_P^2}\left(\hat{p}_b\left[\hat{b}, \hat{H}\right] + \left[\hat{b}, \hat{H}\right]\hat{p}_b\right) - \frac{1}{4i\gamma\ell_P^2}\left(\hat{c}[\hat{p}_c, \hat{H}] + [\hat{p}_c, \hat{H}]\hat{c}\right).\end{aligned} \tag{31}$$

From Section 2.2, for kets, bras, and inner products in the Bohr representation, we use no subscript. For kets, bras, and inner products in the Schrödinger representation, we use the subscript S:

$$\langle \psi, \phi \rangle_S := \int \overline{\psi(b,c)}\phi(b,c)db\,dc.$$

Given a function $\phi(b,c)$, its interpretation as a quantum state is independent of whether one uses the Schrödinger or Bohr representations, so $|\phi\rangle = |\phi\rangle_S$, whereas its interpretation as a linear functional on states depends on the inner product, so $\langle\phi| \neq {}_S\langle\phi|$. The strategy is to recast Equation (31) in terms of the matrix elements of $\hat{H}$ in the Schrödinger representation on the $|p_b', p_c'\rangle_S = |p_b', p_c'\rangle$ basis, where the action of the position operators is given by

$$ {}_S\langle p_b', p_c'|\hat{b} = i\gamma\ell_P^2 \frac{\partial}{\partial p_b'}\, {}_S\langle p_b', p_c'|$$
$$ {}_S\langle p_b', p_c'|\hat{c} = 2i\gamma\ell_P^2 \frac{\partial}{\partial p_c'}\, {}_S\langle p_b', p_c'|,$$

and their conjugates. We have

$$
\begin{aligned}
(n+1)\,{}_{\rm S}\langle p_b'', p_c''|\hat{H}|p_b', p_c'\rangle_{\rm S} &= \frac{1}{2i\gamma\ell_P^2}\,{}_{\rm S}\Big\langle p_b'', p_c''\Big|\hat{p}_b\hat{b}\hat{H} - \hat{p}_b\hat{H}\hat{b} + \hat{b}\hat{H}\hat{p}_b - \hat{H}\hat{b}\hat{p}_b\Big|p_b', p_c'\Big\rangle_{\rm S} \\
&\quad - \frac{1}{4i\gamma\ell_P^2}\,{}_{\rm S}\Big\langle p_b'', p_c''\big|\hat{c}\hat{p}_c\hat{H} - \hat{c}\hat{H}\hat{p}_c + \hat{p}_c\hat{H}\hat{c} - \hat{H}\hat{p}_c\hat{c}\big|p_b', p_c'\Big\rangle_{\rm S} \\
= \frac{1}{2}\left(p_b''\frac{\partial}{\partial p_b''} - p_b''\left(-\frac{\partial}{\partial p_b'}\right) + \frac{\partial}{\partial p_b''}p_b' - p_b'\left(-\frac{\partial}{\partial p_b'}\right)\right)&{}_{\rm S}\langle p_b'', p_c''|\hat{H}|p_b', p_c'\rangle_{\rm S} \\
- \frac{1}{2}\left(\frac{\partial}{\partial p_c''}p_c'' - \frac{\partial}{\partial p_c''}p_c' + p_c''\left(-\frac{\partial}{\partial p_c'}\right) - \left(-\frac{\partial}{\partial p_c'}\right)p_c'\right)&{}_{\rm S}\langle p_b'', p_c''|\hat{H}|p_b', p_c'\rangle_{\rm S} \\
= \left(\frac{1}{2}(p_b' + p_b'')\left(\frac{\partial}{\partial p_b'} + \frac{\partial}{\partial p_b''}\right) - \frac{1}{2}(p_c'' - p_c')\left(\frac{\partial}{\partial p_c''} - \frac{\partial}{\partial p_c'}\right) - 1\right)&{}_{\rm S}\langle p_b'', p_c''|\hat{H}|p_b', p_c'\rangle_{\rm S}\,.
\end{aligned} \tag{32}
$$

Making the change of variables

$$
\begin{aligned}
u_b &= p_b' + p_b'', \quad & v_b &= p_b'' - p_b' \\
u_c &= p_c' + p_c'', \quad & v_c &= p_c'' - p_c'
\end{aligned}
$$

and defining

$$
f(u_b, v_b, u_c, v_c) := {}_{\rm S}\langle p_b'', p_c''|\hat{H}|p_b', p_c'\rangle_{\rm S}\,,
$$

this becomes

$$
\left(u_b\frac{\partial}{\partial u_b} - v_c\frac{\partial}{\partial v_c}\right)f(u_b, v_b, u_c, v_c) = (n+2)f(u_b, v_b, u_c, v_c). \tag{33}
$$

Now, for a general path $(u_b(s), v_b(s), u_c(s), v_c(s))$ in the parameter space, we have

$$
\frac{df}{ds} = \frac{\partial f}{\partial u_b}\frac{du_b}{ds} + \frac{\partial f}{\partial v_b}\frac{dv_b}{ds} + \frac{\partial f}{\partial u_c}\frac{du_c}{ds} + \frac{\partial f}{\partial v_c}\frac{dv_c}{ds}.
$$

As long as the chosen path satisfies $\frac{du_b}{ds} = u_b$, $\frac{du_c}{ds}, \frac{dv_b}{ds} = 0$, and $\frac{dv_c}{ds} = -v_c$, which is equivalent to

$$
\begin{aligned}
&u_b(s) = C_b e^s, \text{ for some } C_b \in \mathbb{R}, \\
&v_c(s) = C_c e^{-s}, \text{ for some } C_c \in \mathbb{R}, \text{ and} \\
&u_c, v_b \in \mathbb{R}, \text{ constant},
\end{aligned}
$$

then Equation (33) then simplifies to

$$
\frac{df}{ds} = (n+2)f
$$

with the general solution

$$
f = Ce^{(n+2)s}.
$$

That is, for all $C_b, v_b, u_c, C_c \in \mathbb{R}$, there exists some real $C(C_b, v_b, u_c, C_c) \in \mathbb{R}$ such that

$$
f(C_b e^s, v_b, u_c, C_c e^{-s}) = C(C_b, v_b, u_c, C_c)e^{(n+2)s} \tag{34}
$$

for all $s \in \mathbb{R}$. In particular, for $s = -\ln|C_b|$, this becomes

$$
f(\mathrm{sgn}(C_b), v_b, u_c, C_c|C_b|) = C(C_b, v_b, u_c, C_c)|C_b|^{-(n+2)}.
$$

Using this to eliminate $C(C_b, v_b, u_c, C_c)$ from Equation (34) and letting $u_b := C_b e^s$ and $v_c := C_c e^{-s}$, we obtain

$$f(u_b, v_b, u_c, v_c) = C_{\mathrm{sgn}(u_b)}(v_b, u_c, v_c|u_b|)|u_b|^{n+2}, \tag{35}$$

where we have defined

$$C_\sigma(v_b, u_c, w) := f(\sigma, v_b, u_c, w).$$

Using the fact that we have assumed $n > -3$, one can check that Equation (35) satisfies Equation (33) with no further restriction. That is, from Equation (35), the general solution to Equation (32) is

$${}_{\mathrm{S}}\langle p_b'', p_c''|\hat{H}|p_b', p_c'\rangle_{\mathrm{S}} = C_{\mathrm{sgn}(p_b''+p_b')}(p_b'' - p_b', p_c'' + p_c', |p_b'' + p_b'|(p_c'' - p_c'))|p_b'' + p_b'|^{n+2} \tag{36}$$

with $C_\sigma(v_b, u_c, w)$ beingarbitrary and real.

4.3. Operator Form of the Solution

From Equation (36), the action of $\hat{H}$ on an arbitrary state $|p_b', p_c'\rangle = |p_b', p_c'\rangle_{\mathrm{S}}$ is

$$\begin{aligned}\hat{H}|p_b', p_c'\rangle &= \int |p_b'', p_c''\rangle_{\mathrm{S}}\ {}_{\mathrm{S}}\langle p_b'', p_c''|\hat{H}|p_b', p_c'\rangle dp_b'' dp_c'' \\ &= \int C_{\mathrm{sgn}(p_b''+p_b')}(p_b'' - p_b', p_c'' + p_c', |p_b'' + p_b'|(p_c'' - p_c'))|p_b'' + p_b'|^{n+2}|p_b'' p_c''\rangle dp_b'' dp_c''.\end{aligned} \tag{37}$$

We define the new variables A and B by

$$\begin{aligned} p_b'' &= p_b' + (p_b'' - p_b') =: p_b' + \gamma\ell_P^2 A \\ p_c'' &= p_c' + \frac{\frac{1}{2}|p_b' + p_b''|(p_c'' - p_c')}{|p_b' + \frac{1}{2}(p_b'' - p_b')|} =: p_c' + \frac{4\gamma\ell_P^4 B}{|p_b' + \frac{1}{2}\gamma\ell_P^2 A|}. \end{aligned} \tag{38}$$

A and B are then given explicitly by

$$A = \frac{p_b'' - p_b'}{\gamma\ell_P^2} \tag{39}$$

$$B = \frac{|p_b'' + p_b'|(p_c'' - p_c')}{8\gamma\ell_P^4}. \tag{40}$$

The reason for this definition will be clear in further steps. Performing the change of variables from (p_b'', p_c'') to (A, B) in the integral Equation (37) gives

$$\begin{aligned}\hat{H}|p_b', p_c'\rangle = \int C'_{\mathrm{sgn}(2p_b'+\gamma\ell_P^2 A)}\left(A, 2p_c' + \frac{4\gamma\ell_P^4 B}{|p_b' + \frac{1}{2}\gamma\ell_P^2 A|}, B\right)|2p_b' + \gamma\ell_P^2 A|^{n+1}\cdot \\ \cdot\left|p_b' + \gamma\ell_P^2 A, p_c' + \frac{4\gamma\ell_P^4 B}{|p_b' + \frac{1}{2}\gamma\ell_P^2 A|}\right\rangle dA dB\end{aligned} \tag{41}$$

where $C'_\sigma(A, u_c, B) := 8\gamma^2\ell_P^2 C_\sigma(\gamma\ell_P^2 A, u_c, 8\gamma\ell_P^4 B)$. This result can then be written by using the action of shift operators as

$$\begin{aligned}&\hat{H}|p_b', p_c'\rangle = \\ &\left(\int e^{\frac{iA}{2}\hat{b}} e^{\frac{iB}{2}\frac{\hat{c}}{|\hat{p}_b|}} |\hat{p}_b|^{n+1}\alpha(A, B, \hat{p}_c, \mathrm{sgn}\, p_b) e^{\frac{iB}{2}\frac{\hat{c}}{|\hat{p}_b|}} e^{\frac{iA}{2}\hat{b}} dA dB\right)|p_b', p_c'\rangle\end{aligned} \tag{42}$$

for $\alpha : \mathbb{R}^3 \times \{\pm 1\} \to \mathbb{C}$, which is an unconstrained parameter function related to C'. If we define the following quantization prescription for any function $f(p_b, p_c)$,

$$\widehat{f(p_b, p_c) e^{i\left(Ab + B\frac{c}{|p_b|}\right)}} := e^{\frac{iA}{2}\hat{b}} e^{\frac{iB}{2}\frac{\hat{c}}{|\hat{p}_b|}} f(\hat{p}_b, \hat{p}_c) e^{\frac{iB}{2}\frac{\hat{c}}{|\hat{p}_b|}} e^{\frac{iA}{2}\hat{b}}, \tag{43}$$

then the Hamiltonian constraint operator takes the form

$$\hat{H} = \int \widehat{|p_b|^{n+1} \alpha(A, B, p_c, \operatorname{sgn} p_b) e^{i\left(Ab + B\frac{c}{|p_b|}\right)}} \, dA dB. \tag{44}$$

4.4. Preservation of the Bohr Hilbert Space

In Section 4.2, we worked in the Schrödinger representation of the quantum algebra of kinematical observables. However, the representation descending from full loop quantum gravity—and in the simpler isotropic case selected by residual diffeomorphism covariance [12,13]—is the representation on the Bohr Hilbert space. In order to ensure that the operator $\hat{H}$ is well defined on this Hilbert space, it must keep at least a subset of it dense with respect to its inner product. More precisely, we require that $\hat{H}$ maps at least one finite linear combination of momentum eigenstates back into the Bohr Hilbert space so that, in particular, for any p_b'', p_c'', there is at most countable p_b', p_c' such that the matrix elements Equation (36) are non-zero. This will be true if and only if the function α appearing in Equation (44) is an at most countable sum of Dirac delta functions over the integration variables A, B,

$$\alpha(A, B, p_c, \operatorname{sgn} p_b) = \sum_k \alpha_k(p_c, \operatorname{sgn} p_b) \delta(A - A_k(p_c)) \delta(B - B_k(p_c)) \tag{45}$$

where the peaks of the Dirac delta functions are allowed to depend on the third continuous parameter, p_c. The Hamiltonian operator then takes the form

$$\hat{H} = \sum_k \widehat{|p_b|^{n+1} \alpha_k(p_c, \operatorname{sgn} p_b) e^{i\left(A_k(p_c) b + B_k(p_c)\frac{c}{|p_b|}\right)}}. \tag{46}$$

5. Discrete Symmetries

The form (46) for the quantum Hamiltonian is the most general that is covariant under the one-parameter family of residual diffeomorphisms. The remaining discrete residual automorphisms of the $SU(2)$ principal bundle are parity maps that preserve the Poisson brackets of the classical theory and so correspond to unitary transformations in the quantum theory. Explicitly,

'b-parity' $\Pi_b : (b, p_b) \mapsto (-b, -p_b)$ is equivalent to an internal gauge rotation of π around the 3-axis, with the corresponding quantum map being given by $\hat{\Pi}_b |p_b', p_c'\rangle := |-p_b', p_c'\rangle$.

'c-parity' $\Pi_c : (c, p_c) \mapsto (-c, -p_c)$ is equivalent to the action of the antipodal map $(\theta, \phi) \mapsto (\pi - \theta, \phi + \pi)$ as a diffeomorphism combined with internal parity along the 3-axis, with the corresponding quantum map being given by $\hat{\Pi}_b |p_b', p_c'\rangle := |-p_b', p_c'\rangle$.

The classical Hamiltonian $H_{c\ell}$ is odd under both of these parities, so we likewise impose that the quantum Hamiltonian $\hat{H}$ be odd under conjugation by the corresponding unitary operators. This, together with the condition that $\hat{H}$ be invariant under Hermitian conjugation, makes up the discrete symmetries to impose on $\hat{H}$.

We define the classical analog of the operator $\hat{H}$ in Equation (46) to be its preimage under our quantization map, namely,

$$H = \sum_k |p_b|^{n+1} \alpha_k(p_c, \operatorname{sgn} p_b) e^{i\left(A_k(p_c) b + B_k(p_c)\frac{c}{|p_b|}\right)}. \tag{47}$$

It is somewhat remarkable and convenient that our quantization map Equation (43), which was naturally suggested by the solution to the quantum residual diffeomorphism covariance condition, additionally (1.) intertwines complex conjugation and Hermitian conjugation ($\hat{H}^\dagger = \hat{\bar{H}}$) and (2.) is covariant with respect to the parity maps ($\hat{\Pi}_b \hat{H} \hat{\Pi}_b = \widehat{\Pi_b^* H}$, $\hat{\Pi}_c \hat{H} \hat{\Pi}_c = \widehat{\Pi_c^* H}$). As a consequence, imposing that $\hat{H}$ be Hermitian and covariant under the quantum parity maps is equivalent to imposing that the classical analog H Equation (47) be real and covariant under the classical parity maps. The most general such H can always be cast in the form

$$\begin{aligned} H =& |p_b|^{n+1} \operatorname{sgn}(p_b p_c) a_0(p_c) \ + \ |p_b|^{n+1} \sum_{k=1}^{M} \Bigg(\alpha_k(p_c, \operatorname{sgn} p_b) e^{i\left(A_k(p_c)b + B_k(p_c)\frac{c}{|p_b|}\right)} \\ & - \ ((b,p_b) \mapsto (-b,-p_b)) \ - \ ((c,p_c) \mapsto (-c,-p_c)) \ + \ c.c. \Bigg) \end{aligned} \tag{48}$$

where the sum is over integers from 1 to M with M being possibly infinite, $a_0(p_c)$ is even and real, $(b, p_b) \mapsto (-b, -p_b)$ denotes the foregoing terms in the large parentheses with the indicated replacement, $(c, p_c) \mapsto (-c, -p_c)$ does so as well, and $c.c.$ denotes the complex conjugate of the foregoing terms, so the number of terms in the large parentheses is eight. Note that, compared to the form (47), the terms above have been relabeled so that each label $k > 0$ corresponds to eight terms for convenience.

Metric Loop Assumption

As discussed in Section 2.2, the functions of the connection with direct quantum analogs are parallel transports along paths. The Hamiltonian constraint is linear in the curvature of the connection, which must, therefore, be quantized by first regularizing the curvature in terms of holonomies around loops. In minisuperspace quantizations such as the present one, the limit in which these loops approach a point is taken by choosing the loops so that they enclose an area equal to the minimal non-zero eigenvalue Δ of the area operator in full loop quantum gravity. As a consequence, the choice of loops depends on the triad; however, more specifically, it depends on the metric determined by the triad. Thus, in the resulting expression for the holonomies and, hence, the regularized constraint, the coefficients $A_k(p_c)$ and $B_k(p_c)$ of the connection components must be even. We call this assumption the metric loop assumption. The consequent symmetry of the coefficients $A_k(p_c)$ and $B_k(p_c)$ is the final discrete symmetry that we consider.

With this assumption, it becomes convenient to decompose each coefficient $\alpha_k(p_c, \operatorname{sgn} p_b)$ into its even and odd parts in each argument, as well as into its real and imaginary parts,

$$\begin{aligned} \alpha_k(p_c, \operatorname{sgn} p_b) =: \frac{1}{8} \Bigg(& \Big(a_k(p_c) + i\tilde{a}_k(p_c) \Big) \operatorname{sgn}(p_b p_c) - \Big(\tilde{b}_k(p_c) + i b_k(p_c) \Big) \operatorname{sgn} p_b \\ & - \Big(\tilde{c}_k(p_c) + i c_k(p_c) \Big) \operatorname{sgn} p_c - d_k(p_c) - i\tilde{d}_k(p_c) \Bigg), \end{aligned} \tag{49}$$

with $a_k, \tilde{a}_k, b_k, \tilde{b}_k, c_k, \tilde{c}_k, d_k, \tilde{d}_k$ being real and even functions of p_c. The terms in the summand in Equation (48) then reduce to only four terms involving sines and cosines, yielding the following more explicit form:

$$\begin{aligned} H =& |p_b|^{n+1} a_0 \operatorname{sgn}(p_b p_c) \ + \ |p_b|^{n+1} \sum_{k=1}^{M} \Bigg(a_k \operatorname{sgn}(p_b p_c) \cos(A_k b) \cos\left(B_k \frac{c}{|p_b|} \right) \\ & + b_k \operatorname{sgn}(p_b) \cos(A_k b) \sin\left(B_k \frac{c}{|p_b|} \right) + c_k \operatorname{sgn}(p_c) \sin(A_k b) \cos\left(B_k \frac{c}{|p_b|} \right) \\ & + d_k \sin(A_k b) \sin\left(B_k \frac{c}{|p_b|} \right) \Bigg) \end{aligned} \tag{50}$$

with $a_k, b_k, c_k, d_k, A_k, B_k$ (thus far arbitrary) being even functions of p_c alone.

6. Classical Asymptotic Behavior

6.1. Naïve Classical Limit and the Limit of Low Curvature

The standard way to define the classical limit (and, indeed, the only one used in the LQC and loop quantum KS literature so far) is to take the limit as the arguments of the exponentials (or sines) go to zero, which is related to an $\ell_P \to 0$ limit of such arguments [18–20,22,23,28,29]. This limit is in fact equivalent to the limit in which the eigenvalues of extrinsic curvature go to zero. To see this, from Equation (2), one can calculate

$$K_a{}^b = \frac{b}{\gamma\,\mathrm{sgn}(p_b)\sqrt{|p_c|}}\partial_a\phi\phi^b + \frac{b}{\gamma\,\mathrm{sgn}(p_b)\sqrt{|p_c|}}\partial_a\theta\theta^b + \frac{\sqrt{|p_c|}c}{\gamma\,\mathrm{sgn}(p_c)|p_b|}\partial_a x x^b,$$

from which one can read off the eigenvalues of the extrinsic curvature, the limit of whose vanishing is then equivalent to the simultaneous limit

$$\mathfrak{b} := \frac{b}{\sqrt{|p_c|}} \to 0 \quad \text{and} \quad \mathfrak{c} := \frac{\sqrt{|p_c|}c}{|p_b|} \to 0, \tag{51}$$

which, for fixed p_c, is equivalent to the vanishing of the arguments of the sines and cosines in Equation (50). As this is equivalent to the definition of the classical limit in all of the prior LQC and loop quantum KS literature, and as the focus of this study is on the consequences of residual diffeomorphism covariance and not the development of a new condition for imposing the classical limit, this is the definition that we use here as well.

However, we would like to point out that this condition is not sufficient because the true regime in which the correct classical limit should be imposed is that of small four-dimensional curvature scalars, a condition that can be satisfied without the extrinsic curvature being small. Indeed, this is what happens at the horizon in Kantowski–Sachs: The eigenvalues of the extrinsic curvature diverge, while the four-dimensional curvature scalars remain small compared to the Planck scale. In fact, we believe that this is the reason why, up to now, $\overline{\mu}$-schemes have failed to have the correct classical limit at the horizon, something that the models [21,23,26,27] improve upon and that we remark upon further in Section 8.3.

Adapting to the limit in Equation (51), one can rewrite the effective Hamiltonian Equation (50) in terms of $\mathfrak{bc}$ by replacing

$$A_k b \mapsto \sqrt{|p_c|}A_k\mathfrak{b} \qquad \text{and} \qquad B_k\frac{c}{|p_b|} \mapsto \frac{1}{\sqrt{|p_c|}}B_k\mathfrak{c}.$$

The classical limit is then obtained by considering the leading terms in the asymptotic expansion in the limit $(\mathfrak{b},\mathfrak{c}) \to (0,0)$.

6.2. Equations for Correct Asymptotic Behavior in the Naïve Classical Limit

When comparing the expanded Hamiltonian with Equation (5), one should ask which terms are relevant to contribute to $H_{c\ell}$ and which are subdominant. The classical Hamiltonian has the form $H_{c\ell} = A \cdot 1 + B\mathfrak{b}^2 + C\mathfrak{bc}$, and the relevance or subdominance relative to each component must be checked separately. Specifically, for given n, m, if

$$\lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{b}^n\mathfrak{c}^m}{1} = \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{b}^n\mathfrak{c}^m}{\mathfrak{b}^2} = \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{b}^n\mathfrak{c}^m}{\mathfrak{bc}} = 0,$$

independently of how the limit is taken, then $\mathfrak{b}^n\mathfrak{c}^m$ is subdominant to each term in H_{cl} in the classical limit; otherwise, we call the term relevant and require the coefficients to match the corresponding ones in $H_{c\ell}$. In particular,

$$
\begin{aligned}
&\mathcal{O}(1): \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{1}{1} = 1 && \Rightarrow \quad \text{Relevant}\\
&\mathcal{O}(\mathfrak{b}): \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{b}}{\mathfrak{b}^2} = \pm\infty && \Rightarrow \quad \text{Relevant}\\
&\mathcal{O}(\mathfrak{c}): \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{c}}{\mathfrak{b}\mathfrak{c}} = \pm\infty && \Rightarrow \quad \text{Relevant}\\
&\mathcal{O}(\mathfrak{b}\mathfrak{c}): \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{b}\mathfrak{c}}{\mathfrak{b}\mathfrak{c}} = 1 && \Rightarrow \quad \text{Relevant}\\
&\mathcal{O}(\mathfrak{b}^2): \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{b}^2}{\mathfrak{b}\mathfrak{c}} = \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{b}}{\mathfrak{c}} = \text{indefinite} && \Rightarrow \quad \text{Relevant}\\
&\mathcal{O}(\mathfrak{c}^2): \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{c}^2}{\mathfrak{b}\mathfrak{c}} = \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{c}}{\mathfrak{b}} = \text{indefinite} && \Rightarrow \quad \text{Relevant}\\
&\mathcal{O}(\mathfrak{b}^2\mathfrak{c}): \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{b}^2\mathfrak{c}}{1} = \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{b}^2\mathfrak{c}}{\mathfrak{b}^2} = \lim_{(\mathfrak{b},\mathfrak{c})\to(0,0)} \frac{\mathfrak{b}^2\mathfrak{c}}{\mathfrak{b}\mathfrak{c}} = 0 && \Rightarrow \quad \text{Subdominant}
\end{aligned}
$$

Every other term of higher order will again be subdominant relative to the terms in $H_{c\ell}$. Therefore, the terms relevant for the classical asymptotic behavior are those proportional to the constant: b, c, bc, b^2, and c^2.

Calling $\Lambda = \frac{(4\pi)^n}{2G\gamma^2}$ for simplicity, we obtain the following system of equations enforcing the correct (naïve) classical limit:

$$
\begin{aligned}
\mathcal{O}(1): &\quad -\Lambda\gamma^2|p_c|^{\frac{n-1}{2}} = a_0 + \sum_{k=1}^{M} a_k\\
\mathcal{O}(\mathfrak{b}): &\quad 0 = \sum_{k=1}^{M} c_k A_k\\
\mathcal{O}(\mathfrak{c}): &\quad 0 = \sum_{k=1}^{M} b_k B_k\\
\mathcal{O}(\mathfrak{b}\mathfrak{c}): &\quad -2\Lambda|p_c|^{\frac{n+1}{2}} = \sum_{k=1}^{M} d_k A_k B_k\\
\mathcal{O}(\mathfrak{b}^2): &\quad 2\Lambda|p_c|^{\frac{n-1}{2}} = \sum_{k=1}^{M} a_k A_k^2\\
\mathcal{O}(\mathfrak{c}^2): &\quad 0 = \sum_{k=1}^{M} a_k B_k^2
\end{aligned}
\tag{52}
$$

6.3. Choice of Lapse

With the notion of the classical limit that was made precise above, it is natural at this point to remark on why we have not included a certain common and usually convenient choice of lapse in our derivations. Classically, this choice of lapse, which decouples the dynamics in the (b, p_b), (c, p_c) parts, is

$$
N = \frac{\gamma}{b}\,\mathrm{sgn}\,(p_c)\sqrt{|p_c|},
\tag{53}
$$

resulting in

$$
H_{c\ell}[N] = -\frac{1}{2G\gamma}\left(p_b\left(b + \frac{\gamma^2}{b}\right) + 2cp_c\right) = H_b[N_{c\ell}] + H_c[N_{c\ell}].
\tag{54}
$$

As convenient as this choice of lapse is, the presence of the $1/b$ factor complicates the definition of a corresponding operator on the Bohr Hilbert space.

Polymerized versions of Equation (54) have indeed been introduced in recent works, yielding effective Hamiltonians that keep the decoupling property [21,23,26]. In [21], for example, this is achieved by replacing $1/b$ with the function

$$f(b) = \frac{\delta_b}{\sin(\delta_b b)} \tag{55}$$

where δ_b is a constant, μ. (In [23,26], the same substitution is made, but with δ_b depending on both b and p_b—see Section 8.3.) As required, this is asymptotically equal to $1/b$ in the classical limit $b \to 0$. Though [21] introduces an operator on the Bohr Hilbert space, it is only for the bare Hamiltonian constraint without a lapse (that is, for a lapse equal to 1)—polymerization of the lapse is only presented in the effective Hamiltonian. In [23], in the note at the end of Appendix A, a strategy is suggested for the construction of a fully quantum Hamiltonian operator but is not carried out.

Nevertheless, as a multiplicative operator, one can in fact show that Equation (55) is densely defined on $\mathcal{H}_{\text{Bohr}}$. For example, if we choose the domain $\mathcal{D} := \sin(\mu b)\mathcal{H}_{\text{Bohr}}$, one can check that

$$\lim_{\epsilon \to 0} \left|\left| e^{i\mu b} - \frac{e^{i\mu b}\sin(\mu b)}{i\epsilon + \sin(\mu b)} \right|\right|_{\text{Bohr}} = 0, \tag{56}$$

so that each element $e^{i\mu b}$ of the momentum basis of $\mathcal{H}_{\text{Bohr}}$ is the limit of a corresponding family $\phi^{\epsilon}_{\mu}(b) := \frac{e^{i\mu b}\sin(\mu b)}{i\epsilon + \sin(\mu b)}$ in $\mathcal{D}$, showing that $\mathcal{D}$ is dense in $\mathcal{H}_{\text{Bohr}}$.

That being said, central to analyses of loop quantizations of symmetry-reduced models is the momentum representation, in which every operator takes the form of a countable linear combination of shift operators with possibly non-constant coefficients. To cast the multiplicative operator $f(b)$ in this form requires its Fourier decomposition, which, since it is periodic, is a series. Since, over a period, $f(b)$ is not square-integrable and, thus, not absolutely integrable, its Fourier series decomposition exists only in the distributional sense, with an infinite number of non-zero terms. Explicitly, if we interpret it as the distribution defined by its Cauchy principal value, since it is odd, its Fourier series decomposition includes only sine terms, with coefficients given by

$$b_n := \frac{2\mu^2}{\pi} \int_0^{\pi/\mu} \frac{\sin(n\mu b)}{\sin(\mu b)} db = \begin{cases} 2\mu & \text{for } n \text{ odd} \\ 0 & \text{for } n \text{ even} \end{cases}, \tag{57}$$

yielding the Fourier series

$$\begin{aligned} \sum_{n=1}^{\infty} b_n \sin(n\mu b) &= 2\mu \lim_{M\to\infty} \sum_{m=1}^{M} \sin((2m+1)\mu b) \\ &= 2f(b) \lim_{M\to\infty} \sin^2((M+1)\mu b) \end{aligned} \tag{58}$$

which converges to $f(b)$ in the distributional sense.

Note, however, that one could also quantize $1/b$ as any periodic function asymptotic to $1/b$ as $b \to 0$. Any such function will again not be square integrable over a period and so will possess an infinite number of terms in its Fourier expansion. Furthermore, for a large class of such functions, an argument similar to that above can be used to show that it is densely defined on $\mathcal{H}_{\text{Bohr}}$—for example, if the function's absolute value is bounded by $\left|\frac{A}{\sin(\mu b)}\right|$ for some A and μ, the argument follows from the above argument for $\frac{\mu}{\sin(\mu b)}$. Thus, there is actually an infinite-dimensional ambiguity in how to quantize $1/b$ on the Bohr Hilbert space: $\widehat{\frac{1}{b}} = \frac{\mu}{\sin \mu b}$ is not the only possible one. To avoid infinite-dimensional ambiguities such as this, we choose to restrict consideration to Hamiltonian operators with only a finite number of shift operators, thereby excluding lapses with dependence on $1/b$.

In the following section, we will consider the even more restrictive requirement that the number of terms in the Hamiltonian operator be minimal.

For other recent works exploring Hamiltonian constraint operators with different lapse functions, see, for example, [30–33].

7. Minimality

Following the motivation of [15], we consider a further requirement: that the Hamiltonian has a minimum number of terms, i.e., a minimum number of shift exponentials consistent with the other requirements imposed. We achieve this by finding the solution of Equation (52) for which the maximal number of coefficients can be set equal to zero. From $\mathcal{O}(\mathfrak{b})$ and $\mathcal{O}(\mathfrak{c})$, this immediately implies that $b_k = c_k = 0$, reducing the system of equations to

$$\begin{aligned} \mathcal{O}(1): &\quad -\Lambda\gamma^2|p_c|^{\frac{n-1}{2}} = a_0 + \sum_{k=1}^{M} a_k \\ \mathcal{O}(\mathfrak{b}\mathfrak{c}): &\quad -2\Lambda|p_c|^{\frac{n+1}{2}} = \sum_{k=1}^{M} d_k A_k B_k \\ \mathcal{O}(\mathfrak{b}^2): &\quad 2\Lambda|p_c|^{\frac{n-1}{2}} = \sum_{k=1}^{M} a_k A_k^2 \\ \mathcal{O}(\mathfrak{c}^2): &\quad 0 = \sum_{k=1}^{M} a_k B_k^2 \end{aligned} \tag{59}$$

The case $M = 1$ is trivially ruled out, since the last equation would require $a_1 = 0$ or $B_1 = 0$, which would be inconsistent with the other equations. Choosing $M = 2$, we first look at $\mathcal{O}(c^2)$:

$$a_1 B_1^2 + a_2 B_2^2 = 0.$$

Since we cannot have both a_1 and a_2 equal to zero (because of the $\mathcal{O}(\mathfrak{b}^2)$ equation), then, if we set $a_1 = 0$, we automatically must have $B_2 = 0$. d_2 then appears nowhere in the remaining equations, so minimality forces $d_2 = 0$. The solution for the remaining parameters is then

$$a_2 = \frac{2\Lambda|p_c|^{\frac{n-1}{2}}}{A_2^2}, \quad d_1 = -\frac{2\Lambda|p_c|^{\frac{n+1}{2}}}{A_1 B_1}, \quad a_o = -\Lambda|p_c|^{\frac{n-1}{2}}\left(\gamma^2 + \frac{2}{A_2^2}\right)$$

for A_1, A_2, B_1 real functions of $|p_c|$ non-vanishing for $|p_c| \neq 0$, but otherwise arbitrary.

The minimal Hamiltonian can then be written as

$$\begin{aligned} H &= -\Lambda|p_b|^{n+1}|p_c|^{\frac{n-1}{2}}\,\mathrm{sgn}(p_b p_c)\left(\left(\gamma^2 + \frac{2}{A_2^2}\right) + 2|p_c|\,\mathrm{sgn}(p_b p_c)\frac{\sin(A_1 b)}{A_1}\frac{\sin\left(B_1\frac{c}{|p_b|}\right)}{B_1} - 2\frac{\cos(A_2 b)}{A_2^2}\right) \\ &= -\frac{V^{n+1}\,\mathrm{sgn}(b)}{8\pi G\gamma^2 p_c}\left(\gamma^2 + 2p_c\,\mathrm{sgn}\,p_b\frac{\sin(A_1 b)}{A_1}\frac{\sin\left(B_1\frac{c}{|p_b|}\right)}{B_1} + \frac{4\sin^2\left(\frac{A_2}{2}b\right)}{A_2^2}\right), \end{aligned} \tag{60}$$

and, using Equation (43), the full Hamiltonian operator becomes

$$\begin{aligned}8\pi G\gamma^2\hat{H} =& \frac{\hat{V}^{(n+1)}\,\mathrm{sgn}(p_b)}{-\hat{p}_c}\left(\gamma^2+\frac{2}{A_2^2}\right)\\ &+e^{\frac{iA_1b}{2}}e^{\frac{iB_1c}{2|p_b|}}\frac{\hat{V}^{(n+1)}}{2A_1B_1}e^{\frac{iB_1c}{2|p_b|}}e^{\frac{iA_1b}{2}}-e^{\frac{iA_1b}{2}}e^{\frac{-iB_1c}{2|p_b|}}\frac{\hat{V}^{(n+1)}}{2A_1B_1}e^{\frac{-iB_1c}{2|p_b|}}e^{\frac{iA_1b}{2}}\\ &-e^{\frac{-iA_1b}{2}}e^{\frac{iB_1c}{2|p_b|}}\frac{\hat{V}^{(n+1)}}{2A_1B_1}e^{\frac{iB_1c}{2|p_b|}}e^{\frac{-iA_1b}{2}}+e^{\frac{-iA_1b}{2}}e^{\frac{-iB_1c}{2|p_b|}}\frac{\hat{V}^{(n+1)}}{2A_1B_1}e^{\frac{-iB_1c}{2|p_b|}}e^{\frac{-iA_1b}{2}}\\ &+e^{\frac{iA_2b}{2}}\frac{\hat{V}^{(n+1)}\,\mathrm{sgn}(p_b)}{A_2^2p_c}e^{\frac{iA_2b}{2}}+e^{\frac{-iA_2b}{2}}\frac{\hat{V}^{(n+1)}\,\mathrm{sgn}(p_b)}{A_2^2p_c}e^{\frac{-iA_2b}{2}}. \end{aligned} \tag{61}$$

8. Comparison with Prescriptions in the Literature

Most proposals for a Hamiltonian in loop quantum Kantowski–Sachs are only for an effective Hamiltonian from which physical predictions can be made [18–20,23–25,34], while a few others seek to build a full Hamiltonian operator [16,17,21,25]. While comparing full Hamiltonian operators may be harder, due to possible differences in the operators' ordering, it is easy to verify whether a proposed effective Hamiltonian matches one of the selected solutions Equation (50) (and whether it is minimal).

What distinguishes each approach to KS is the prescription for quantizing the curvature and connection factors in the Hamiltonian constraint—specifically, how the curves used to regularize these factors are determined by the edges, coordinates, or metric of the fiducial cell in terms of the smallest non-zero area eigenvalue Δ. The coordinate lengths of the components of these curves are what determine the coefficients of the connection components in the exponentials appearing in the final effective Hamiltonian constraint. From the form (46), we see that diffeomorphism covariance forces some of these coefficients to be non-constant—specifically, the coefficient of c must depend inversely on p_b, a fact that can be seen more directly from the flows in Equation (25). μ_0-schemes [16–18,21,34] for which all such coordinate edge lengths are constant are, thus, excluded by covariance. Instead, covariance points towards some sort of $\bar{\mu}$-scheme, as in [19,20]. In the first two subsections below, we specify the relation of such proposals to our results. In the last two subsections, we then discuss other proposals in the literature with non-constant coordinate edge lengths.

8.1. $n = 0$: Proper Time Case

If we take $N = 1$—which is equivalent to $n = 0$ in the lapse Equation (6)—$A_1 = \sqrt{\frac{\Delta}{|p_c|}}$, $A_2 = 2A_1$, and $B_1 = \sqrt{|p_c|\Delta}$, we obtain

$$H = -\frac{|p_b|\sqrt{|p_c|}}{2G\gamma^2\Delta}\left(\frac{\gamma^2\Delta}{|p_c|}+2\sin\left(\sqrt{\frac{\Delta}{|p_c|}}b\right)\sin\left(\sqrt{|p_c|\Delta}\frac{c}{|p_b|}\right)+\sin^2\left(\sqrt{\frac{\Delta}{|p_c|}}b\right)\right), \tag{62}$$

which matches the results obtained by Joe and Singh in [20] and Cortez, Cuervo, Morales-Técotl and Ruelas in [22] for $p_b, p_c > 0$.

8.2. $n = 1$: Harmonic Time Gauge

For $n = 1$, with the same assumptions and restrictions as above, we find

$$H = -\frac{2\pi p_b^2 p_c}{G\gamma^2\Delta}\left(\frac{\gamma^2\Delta}{p_c}+2\sin\left(\sqrt{\frac{\Delta}{p_c}}b\right)\sin\left(\sqrt{p_c\Delta}\frac{c}{p_b}\right)+\sin^2\left(\sqrt{\frac{\Delta}{p_c}}b\right)\right), \tag{63}$$

matching the result obtained by Chiou in [19].

8.3. AOS Prescription

Differently from the above cases is what was recently introduced by Ashtekar, Olmedo, and Singh (AOS) [23,26]. As usual, when constructing the Hamiltonian for loop quantum Kantowski–Sachs, they begin by regularizing the curvature in terms of parallel transports around finite loops, with edges in the x-direction with coordinate lengths $L_o\delta_c$ and edges within x =constant surfaces along geodesics of the fiducial unit sphere metric $d\Omega^2 = d\theta^2 + \sin^2\theta d\phi^2$ with (dimensionless) 'lengths' $2\pi\delta_b$ relative to $d\Omega^2$. The key requirements in this model are the following:

1. (as in [21,27]) δ_b and δ_c are Dirac observables—i.e., are constant on dynamical trajectories;
2. at the transition surface that replaces the classical singularity, the regularizing loops enclose a physical area equal to the area gap Δ when the Hamiltonian constraint is satisfied.

In the resulting effective model, the expansion and shear diverge at the horizon, just as in classical general relativity, so the model matches general relativity in this regime, exactly as it should. This is a major advantage of AOS over the $\overline{\mu}$-schemes introduced so far, an advantage shared by [21,27], suggesting that it is the first of the above requirements that ensures this. In contrast to [21,27], the AOS model further ensures, as in the $\overline{\mu}$-schemes, that the transition surface always occurs in a regime where quantum gravity effects are expected to be relevant, namely, when the Kretschmann scalar is on the order of the Planck scale. In addition to these advantages that no other model simultaneously shares, the authors of [23,26] extended their analysis to the exterior of the black hole and explored the global structure of the resulting maximally extended effective space-time. It is, thus, the most well-developed and physically viable model proposed so far in the literature.

Conditions 1. and 2. still leave considerable freedom in the definitions of δ_b and δ_c, and there is also freedom in the choice of lapse. The authors choose to use these freedoms in order to decouple the dynamics of the (b, p_b) and (c, p_c) degrees of freedom, allowing for exact analytic solutions to the effective equations. Specifically, the lapse Equation (53) is the choice made by AOS. With this choice, the regularized effective Hamiltonian constraint becomes

$$H = -\frac{1}{2G\gamma}\left[\left(\frac{\sin(\delta_b b)}{\delta_b} + \frac{\gamma^2\delta_b}{\sin(\delta_b b)}\right)p_b + 2\frac{\sin(\delta_c c)}{c}p_c\right]. \tag{64}$$

In order for this effective Hamiltonian to retain the decoupling of the b and c degrees of freedom in the classical theory, they further require that

$$\delta_b \text{ depend only on } (b, p_b) \text{ and } \delta_c \text{ only on } (c, p_c). \tag{65}$$

As convenient as it is to have an exactly soluble model, the choice of lapse and the conditions in Equation (65), respectively, come at the cost of (a.) the corresponding Hamiltonian constraint operator having an infinite number of shift terms if implemented on the usual Bohr Hilbert space motivated by loop quantum gravity and (b.) the effective Hamiltonian constraint not being covariant under residual diffeomorphisms. That the corresponding operator on the Bohr Hilbert space must have an infinite number of shift operators follows from our discussion in Section 6.3.

To see (b.), we must be more explicit. Concretely, in AOS, in the large-mass limit, one can understand $\delta_b(b, p_b)$ as being obtained as the solution of the transcendental system of two equations consisting of the first equation in each of (2.12) and (2.13) in [26], and $\delta_c(c, p_c)$ is obtained as the solution of the system consisting of the second equation in each of these. By using (2.13) to eliminate m_b in (2.12), one sees that not only can δ_b depends only on b and p_b, but it must depend on both non-trivially. Likewise, δ_c must depend on both c and p_c non-trivially. As a consequence, under the flow in Equation (25), the argument of the first sine in Equation (64) is non-constant, $(\dot{\delta_b b}) = \frac{\partial \delta_b}{p_b} p_b b \neq 0$, forcing the effective AOS Hamiltonian to be not covariant under residual diffeomorphisms.

Note that, even without the specific prescription of AOS for fixing $\delta_b(b, p_b)$ and $\delta_c(c, p_c)$, the assumption in Equation (65) alone is enough to force incompatibility with the form in Equation (47), which we have shown is required by residual diffeomorphism covariance and preservation of the Bohr Hilbert space, in which δ_c must depend on p_b with a very specific dependence. This suggests that the desire to maintain decoupling of the b and c degrees of freedom in the effective theory, as convenient as it is, is incompatible with simultaneous residual diffeomorphism covariance and the existence of a corresponding operator preserving the Bohr Hilbert space. That is, if one desires both of the latter two properties, then the b and c degrees of freedom are forced to interact.

It must be emphasized that, even though the precise effective Hamiltonian constraint of AOS is not covariant under residual diffeomorphisms, the key physical predictions calculated so far, such as the universal upper bound on all scalar curvatures, are invariant under residual diffeomorphisms. Furthermore, the works [23,26] never suggest that their proposed effective Hamiltonian has a corresponding quantum operator on the Bohr Hilbert space. Indeed, they explicitly mention the construction of a corresponding operator and associated Hilbert space as an open problem at the end of Appendix A in [23], and they provide a strategy for constructing an alternative quantum framework.

However, with diffeomorphism symmetry being the basic symmetry of gravity, there is good motivation to seek an effective Hamiltonian that is exactly covariant under residual diffeomorphisms. Because of this, it might be valuable to attempt a modification of AOS in which the condition in Equation (65) and, hence, the decoupling of the two degrees of freedom are dropped and in which such exact covariance is imposed in its place. Such a model would be mathematically more complex but, potentially, more physically compelling, including all of the physically compelling features of AOS, as well as the exact residual diffeomorphism covariance of the $\overline{\mu}$ models.

8.4. Newer Proposals

Some newer proposals with different approaches are worth mentioning:

- Assanioussi and Mickel [29] proposed an effective Hamiltonian constructed via regularized Thiemann identities in the $\bar{\mu}$ scheme. Their starting point differs from ours—the Hamiltonian is from the full theory, with a Euclidian and a Lorentzian component, while our approach uses the symmetry-reduced Hamiltonian Equation (5), in which these two terms are not distinguished—so the final result is expected to be different. However, their result does lie in the family in Equation (50) selected by using residual diffeomorphism covariance and discrete symmetries, and our minimal result has the same form as the Euclidian part calculated by them.
- Bodendorfer, Mele, and Munch [28] introduce new pairs of canonical variables,

  $$v_k := \frac{\gamma p_b |p_c|}{2^{\frac{14}{3}} b}, \qquad v_j := \frac{p_b}{8b}(c p_c - b p_b), \qquad k := \frac{2^{\frac{11}{3}} bc}{\gamma^2 p_b \operatorname{sgn} p_c}, \qquad j := \frac{4b}{\gamma p_b},$$

  in order to have a relation $\mathcal{K} \propto k^2$ for the Kretschmann scalar, inspired by the relation $R \propto b^2$ that appears using (b, v) variables in the homogeneous isotropic case. They use the lapse Equation (53), and the effective Hamiltonian density is obtained through a polymerization of the variables k and j, resulting in

  $$\mathcal{H}_{eff} = 3 v_k \frac{\sin(\lambda_k k)}{\lambda_k} \frac{\sin(\lambda_j j)}{\lambda_j} + v_j \frac{\sin^2(\lambda_j j)}{\lambda_j}.$$

  However, both v_j and v_k are proportional to $1/b$, which requires an infinite number of terms to be represented in the Bohr Hilbert space, as discussed in Section 6.3. Moreover, in order to ensure the covariance of the effective Hamiltonian under the rescaling of the fiducial cell by a factor α, the parameter λ_j—a constant in phase space—is defined to scale as $\lambda_j \mapsto \alpha\lambda_j$. While such a definition is possible to ensure covariance under passive residual diffeomorphisms, there is no such freedom for active diffeomorphisms—arising from a flow in the phase space—where constants are simply constant. As a consequence, their effective Hamiltonian is not covariant under active residual diffeomorphisms, explaining why it does not fall into the class Equation (50) that we selected above. Also, k is quadratic in components of the connections, so the first term in their Hamiltonian could not come from parallel transports of the Ashtekar–Barbero connections. The fact that components of the Ashtekar–Barbero connection appear quadratically in one of the sines furthermore means that the Fourier transform of their effective Hamiltonian with respect to b and c must have uncountable support, impeding a corresponding operator from being densely defined on the usual Bohr Hilbert space reviewed in Section 2.2.

- Sartini and Geiller [25] consider KS with a cosmological constant incorporated via the unimodular formulation of gravity [35], the main motivation being to solve the problem of time without introducing scalar matter. They propose the change of variables

$$p_1 := -\frac{c}{2\gamma}, \qquad v_1 := p_c, \qquad p_2 := \frac{4b}{\gamma p_b}, \qquad v_2 := -\frac{p_b^2}{8}.$$

For their effective theory, they again choose the lapse Equation (53) and polymerize p_1 and p_2, resulting in

$$H = 2\frac{\sin(\lambda_1 p_1)}{\lambda_1}v_1 + \frac{\sin(\lambda_2 p_2)}{\lambda_2}v_2 - 2(1-\Lambda v_1)\frac{\lambda_2}{\sin(\lambda_2 p_2)}. \tag{66}$$

with λ_i constants on phase space. The case here is similar to the one above, where their definition of how the constants λ_i should rescale under changes of the fiducial cell make the effective Hamiltonian covariant under passive but not active diffeomorphisms.

The use of the classical lapse Equation (53) for the effective theory means that, if the effective Hamiltonian would arise from a quantum operator, then the discussion of Section 6.3 would apply again. However, when proposing a quantum Hamiltonian operator, the authors make use of a different lapse, the one corresponding to the use of a unimodular clock, matching Equation (6) for $n = -1$. The Hilbert space on which the non-cosmological constant part of their operator acts is the usual Bohr Hilbert space. That being said, the polymerization of the connection variables in their operator remains the same as in their effective theory and, thus, is again not covariant under active residual diffeomorphisms, so the non-cosmological constant part of the operator is not in the family in Equation (50) that we selected.

9. Conclusions

In this work, we were able to derive a family of Hamiltonian operators for the loop quantum Kantowski–Sachs framework by imposing the quantum analog of covariance under residual diffeomorphisms, as well as other physical criteria. In doing this, we avoided choosing a specific quantization prescription a priori.

We further demonstrated that, for each choice of lapse, the requirement of minimality, that is, a minimal number of shift operators in the Hamiltonian constraint operator—a form of Occam's razor—leads to a family of models parameterized by three functions of p_c. For specific values of these parameters, the model matches proposals in the literature constructed with traditional quantization methods—specifically, the $\overline{\mu}$-prescriptions obtained by Chiou [19] and Joe and Singh [20]. We emphasize, however, that the minimality principle is trustworthy only inasmuch as the other conditions imposed are complete—in particular, we impose no conditions relating the model's dynamics to a choice of full theory dynamics, a condition whose incorporation would likely force a non-minimal choice, as defined here.

We also remarked on the relation of our work to other models in the literature, with particular attention to that of of Ashtekar, Olmedo, and Singh (AOS) [23,26]. First, and most importantly, AOS, as well as [21,27], improved upon all previous works in that the classical limit is correctly imposed at the horizon—a regime where (for macroscopic black holes) curvature is low compared to the Planck scale, so no significant deviation from classical general relativity is expected. That prior models, including those using $\overline{\mu}$-schemes, failed to do this highlights that the condition for the correct classical limit imposed in the literature up until now—and that used in the present paper—is not sufficient. Specifically, the usual condition that the arguments of complex exponentials or, equivalently, of the sine functions go to zero, motivated by a naïve $\ell_P \to 0$ limit and equivalent to eigenvalues of extrinsic curvature going to zero, is neither a necessary nor sufficient condition that space-time curvature scalars go to zero.

The AOS model additionally makes two choices to decouple the evolution of the two degrees of freedom of the model, rendering the dynamics exactly soluble: The choice of lapse and the requirement that δ_b and δ_c depend, respectively, only on the b and c degrees of freedom. As attractive as exact solubility is, the latter of these choices forces the effective Hamiltonian to not be exactly diffeomorphism-covariant. The first of these choices forces the corresponding Hamiltonian constraint operator, if defined on the Bohr Hilbert space motivated by loop quantum gravity, to include an infinite number of shift operators.

It must be emphasized that the key physical predictions of AOS are covariant under residual diffeomorphisms. Nevertheless, we argue that exact diffeomorphism covariance of the full Hamiltonian is a compelling property and that it should be possible to modify the AOS model to require such exact covariance if one gives up decoupling the two degrees of freedom of the model while retaining all of the model's physically compelling features. One systematic path to finding such a new model might be to use the program of the present work but while replacing the usual naïve classical limit used in Section 6.1 with an appropriate corrected condition based on four-dimensional curvature scalars.

Author Contributions: All authors have contributed equally to all aspects of this work. All authors have read and agreed to the published version of the manuscript.

Funding: This work was funded in part by U.S. National Science Foundation Grants PHY-1806290 and PHY-2110234.

Data Availability Statement: Data are contained within the article.

Acknowledgments: The authors thank Christopher Beetle for the discussions, which were helpful in obtaining the results presented in Section 6.3.

Conflicts of Interest: The authors declare no conflicts of interest.

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