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# Quantum isotropy and the reduction of dynamics in Bianchi I

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#### **Abstract**

The authors previously introduced a diffeomorphism-invariant definition of a homogeneous and isotropic sector of loop quantum gravity (LQG), along with a program to embed loop quantum cosmology (LQC) into it. The present paper works out that program in detail for the simpler, but still physically non-trivial, case where the target of the embedding is the homogeneous, but not isotropic, Bianchi I model. The diffeomorphism-invariant conditions imposing homogeneity and isotropy in the full theory reduce to conditions imposing isotropy on an already homogeneous Bianchi I spacetime. The reduced conditions are invariant under the residual diffeomorphisms still allowed after gauge fixing the Bianchi I model. We show that there is a unique embedding of the quantum isotropic model into the homogeneous quantum Bianchi I model that (a) is covariant with respect to the actions of such residual diffeomorphisms, and (b) intertwines both the (signed) volume operator and at least one directional Hubble rate. That embedding also intertwines all other operators of interest in the respective loop quantum cosmological models, including their Hamiltonian constraints. It thus establishes a precise equivalence between dynamics in the isotropic sector of the Bianchi I model and the quantized isotropic model, and not just their kinematics. We also discuss the adjoint relationship between the embedding map defined here and a projection map previously defined by

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Ashtekar and Wilson-Ewing. Finally, we highlight certain features that simplify this reduced embedding problem, but which may not have direct analogues in the embedding of homogeneous and isotropic LQC into full LQG.

Keywords: loop quantum gravity, loop quantum cosmology, diffeomorphism covariance

#### 1. Introduction

Quantum gravity is a domain of physics in which contact with observation remains a challenge, due to the extreme nature of the Planck scale where effects of the corresponding theory are expected to become relevant. That being said, due to cosmic expansion, the entire visible Universe was once Planck sized. Indeed, cosmology has emerged as a promising domain in which to observe potential effects of quantum gravity [1–4], and perhaps such effects have even already been observed [5, 6].

Loop quantum gravity (LQG) [7–10] is a minimalist approach to a theory of quantum gravity guided foremost by Einstein's general principle of relativity, which in modern times is reformulated as diffeomorphism covariance, or background independence. Loop quantum cosmology (LQC) [11–13] is a quantization of the homogeneous isotropic sector of gravity using the same techniques as LQG. To derive the effects of LQG on cosmology, the nearly exact homogeneity and isotropy of the early Universe is exploited by using LQC for calculations. The relative simplicity of LQC allows for exact solutions to dynamics as well as the construction of a complete set of Dirac observable operators.

One can ask whether LQC, a quantization of a symmetry reduced sector of gravity, accurately reflects the physics of full LQG. When the choices made in the quantizations of a field theory and its corresponding symmetry-reduced model are chosen to be appropriately compatible, symmetry reduction and quantization can indeed commute [14]. In order to ask whether LQC reflects the appropriate sector of LQG, one must first specify what this sector is. It should be the quantum analogue of the homogeneous isotropic sector of classical gravity—that is, it should be the space of states in LQG which are homogeneous and isotropic in some sense which is compatible with the diffeomorphism invariance of the theory. A proposal for such a sector has been defined in the prior work [15, 16] by finding diffeomorphism covariant phase space functions on the full gravity phase space whose vanishing is equivalent to the condition of homogeneity and isotropy with respect to some maximal symmetry group on the spatial slice—the symmetry conditions. These phase space functions are furthermore readily quantizable on the LQG Hilbert space, so that the simultaneous kernel of the corresponding operators defines the desired sector in question. The second step is to find some *embedding* of LQC states into the states of this sector. The work [15, 16] did this for a non-interacting toy example and sketched how to embed LQC into full LQG.

The value of constructing an embedding of LQC into full LQG is not simply to both clarify the meaning of homogeneous isotropic in LQG as well as to understand how well LQC represents the physics of this sector. The value, more importantly, lies in its potential to associate each quantization choice in the full theory with a corresponding choice in the reduced theory. With such an association in hand, contact between LQC and observation can provide not only a test of LQG, but can also guide choices made in quantizing the full theory. There are a number of programs which have been introduced to establish such an association [12, 17–23]. The advantages of the present program are that (1) it is compatible with the

dynamics in the full theory, in the sense that diffeomorphism covariance is left intact without gauge fixing, (2) it is compatible with the full space of states in LQG, in the sense that one does not need to restrict to states with support in a lattice, and (3) it potentially establishes a relation with LQC as an exact quantum theory, rather than as an effective theory. Since the so-called ' $\overline{\mu}$ -scheme' in LQC arises from requirements of diffeomorphism covariance [12, 24, 25], it is reasonable to hope that the first two of the above properties of the present strategy will enable a derivation of the  $\overline{\mu}$ -scheme from full LQG without inserting it by hand, in contrast to other approaches up until now. Still, we expect there to be a relation between the approach followed here and at least the approaches of [17, 22]: the map from LQC states to (gauge-fixed, lattice-truncated) LQG states implicit in these latter approaches are based on coherent states, and the range of this implicit embedding is the span of all coherent states with homogeneous isotropic labels. This space is precisely the simultaneous kernel of quantum operators corresponding to the 'holomorphic part' of the appropriate symmetry conditions [14, 26], which are complex in a way exactly analogous to the complex symmetry conditions considered in the strategy of the present work.

The goal of the present paper is to complete the program of [15, 16], but in the simpler case of embedding LQC into *Bianchi I* LQC [27–29], in which homogeneity, but not isotropy, holds *a priori*. The goal of doing this is to see how the program can be carried out to completion in this simpler, but still realistic case, thereby solidifying confidence in the program as well as providing an opportunity to gain intuition that will aid in applying it to embed into full LQG. The results turn out to be cleaner, more satisfactory, and more revealing than we had expected.

In the Bianchi I model, the fully diffeomorphism-invariant condition imposing homogeneity and isotropy introduced in [15, 16] reduces to a *residual* diffeomorphism-invariant condition imposing only *isotropy*, which can be easily quantized in a manner similar to that suggested in [15, 16] for the full theory. We furthermore find that there exists a unique embedding from isotropic to Bianchi I LQC states that is covariant with respect to (canonical) residual diffeomorphisms, and also intertwines the operators in the two theories corresponding to the signed volume and a single directional Hubble rate. This uniquely determined embedding has image contained in the kernel of the quantum isotropy conditions. It furthermore intertwines the Hamiltonian constraints in the two theories, as well as all physically meaningful operators. Interestingly, it is precisely the adjoint of the projection from Bianchi I to isotropic LQC proposed by Ashtekar and Wilson-Ewing in [28].

The rest of this paper is organized as follows. In section 2 we review the Bianchi I model as defined by Ashtekar and Wilson-Ewing in [28]. We then derive in section 3 the restriction, to the Bianchi I phase space, of the constraints proposed in [15] imposing diffeomorphism invariant homogeneity and isotropy. The Poisson brackets of these symmetry conditions among themselves are calculated with an eye toward quantum theory. The general quantization strategy presented in [28] is then used to provide symmetry constraint operators on the Bianchi I Hilbert space, whose simultaneous kernel defines the 'quantum isotropic sector' of Bianchi I. Section 3 ends with a review of the isotropic model. In section 4, we derive the embedding of this model into the quantum isotropic sector of Bianchi I, and exhibit its properties. The successes of the results are sufficiently surprising that we devote section 5 to clarifying the classical origins of these successes. Lastly we close with a discussion.

#### 2. Review of Bianchi I

#### 2.1. Classical theory

The spacetime metric in the Bianchi I model has the form

$$ds^{2} = -N^{2}(t) dt^{2} + a_{y}^{2}(t) dx^{2} + a_{y}^{2}(t) dy^{2} + a_{z}^{2}(t) dz^{2}.$$
 (1)

The natural (co-)triad field on a homogeneous slice of constant t is

$$e_a^i(t) := a_i(t) \stackrel{\circ}{e}_a^i, \quad \text{where } \stackrel{\circ}{e}_a^i := dx_a^i$$
 (2)

is the fiducial (co-)triad. Note that there is no sum over the index i in this definition of  $e_a^i$ . We will write all such sums explicitly. Meanwhile, the extrinsic curvature of a homogeneous slice is

$$K_{ab}(t) = \frac{1}{2} \mathcal{L}_u \, q_{ab}(t) = \sum_i \frac{a_i(t) \, \dot{a}_i(t)}{N(t)} \, \dot{e}_a^i \, \dot{e}_b^i, \tag{3}$$

where  $u = \frac{1}{N(t)} \frac{\partial}{\partial t}$  is the future-directed, unit normal to the homogeneous slice. We will omit any explicit *t*-dependence below.

Geometrically, the spatial coordinates  $x^i$  in (1) can be defined as affine parameters along three mutually orthogonal congruences of parallel geodesics in the Euclidean spatial geometry of the Bianchi I model. Moreover, the directions of those congruences are fixed in (3) to coincide with the principal axes of the extrinsic curvature tensor  $K_{ab}$ . Given appropriate Cauchy data for the Bianchi I model, consisting of a Euclidean spatial metric  $q_{ab}$  and a homogeneous extrinsic curvature  $K_{ab}$ , the spatial coordinates so defined are unique up to (a) affine reparameterizations  $\varphi_{(\mathbf{m},\mathbf{b})}: x^i \mapsto \tilde{x}^i := m_i \, x^i + b^i$  of each congruence, with each  $m_i \neq 0$ , and (b) permutations  $\varphi_\pi: x^i \mapsto \tilde{x}^i := x^{\pi(i)}$  of the coordinate axes, with  $\pi \in S_3$ . Any choice of such coordinates defines a canonical diffeomorphism from the spatial slice to  $\mathbb{R}^3$ . The present coordinate ambiguity therefore reflects the restricted diffeomorphism group  $\overline{\mathrm{Diff}} \approx (S_3 \ltimes \mathbb{R}^3_\times) \ltimes \mathbb{R}^3$  mapping  $\mathbb{R}^3$  to itself, i.e. the group of spatial diffeomorphisms that preserve the partial gauge-fixing conditions implicit in (1) and (3).

The loop quantization of general relativity originates in the Ashtekar formulation of the classical theory. The basic variables of that formulation are the densitized triad

$$E_i^a := |\det e| e_i^a = \frac{|a_x a_y a_z|}{a_i} \mathring{E}_i^a, \tag{4}$$

and the Ashtekar connection with Barbero–Immirzi parameter  $\gamma$ . The latter is given by

$${}^{\gamma}A_a^i := \Gamma_a^i + \gamma K_{ab}e^{bi} = \frac{\gamma \dot{a}_i}{N} \dot{e}_a^i, \tag{5}$$

where  $\Gamma_a^i$  is the spin connection form for  $e_i^a$ , relative to a flat reference connection. Spatial geometry is already flat in the Bianchi I model, so it is simplest to choose the reference connection to be the spin connection, whence  $\Gamma_a^i=0$ . The symplectic structure in Ashtekar gravity generally has the form

$$\Omega(\delta_1, \delta_2) := \frac{2}{\kappa \gamma} \int_{\mathcal{V}} \delta_{[1}{}^{\gamma} A_a^i \, \delta_{2]} E_i^a, \tag{6}$$

where  $\kappa = 8\pi G_{\text{Newton}}$ . The integral in (6) diverges when the field perturbations involved are homogeneous and the spatial slice V is not compact. But, precisely due to that homogeneity,

it then makes sense to restrict the integral to a compact fiducial cell  $\mathcal{V}$ , i.e. to a finite, rectangular volume with edges parallel to the coordinate axes [28]. The symplectic structure then reduces to

$$\Omega = \frac{1}{\kappa \gamma} \sum_{i} dc^{i} \wedge dp_{i}, \tag{7}$$

where we have introduced the reduced phase space coordinates  $(c^i, p_i)$  such that

$$^{\gamma}A_a^i =: c^i \frac{\mathring{e}_a^i}{L_i} \quad \text{and} \quad E_i^a =: \frac{L_i}{L_x L_y L_z} p_i \mathring{E}_i^a.$$
 (8)

The coordinate lengths  $L_i := |\Delta x^i|$  of the edges of the fiducial cell  $\mathcal{V}$  enter these definitions to render the canonical coordinates independent of the initial choice of adapted coordinates  $x^i$  in (1). It will be convenient to exclude those points of the phase space corresponding to degenerate spatial geometries, i.e. having one or more of the  $p_i$ , and hence the volume, equal to zero. Such points are irrelevant in the usual limit used to make predictions, namely that of large fiducial cell volume, corresponding to removal of the infrared regulator [11, 24]. Our Bianchi I phase space is therefore  $\Gamma \cong \mathbb{R}^3 \times \mathbb{R}^3_{\times}$  topologically, where the second factor excludes the three coordinate planes in  $\mathbb{R}^3$  where at least one  $p_i$  vanishes.

Now we consider the transformations of the Bianchi I phase space induced by the restricted spatial diffeomorphisms described above. The phase-space transformation associated with a diffeomorphism  $\varphi_{(\mathbf{m},\mathbf{b})}$  mapping each coordinate axis to itself follows immediately from the pull-backs

$$\varphi_{(\mathbf{m},\mathbf{b})}^* \mathring{e}_a^i = m_i \mathring{e}_a^i \leadsto \varphi_{(\mathbf{m},\mathbf{b})} : (c^i, p_i) \mapsto (\tilde{c}^i, \tilde{p}_i) := \left( m_i c^i, \frac{|m_x m_y m_z|}{m_i} p_i \right). \tag{9}$$

The translation parameter **b** in  $\varphi_{(\mathbf{m},\mathbf{b})}$  has no effect in phase space, as one would expect for a homogeneous model. The situation is slightly more complicated for the diffeomorphisms  $\varphi_{\pi}: \mathbb{R}^3 \to \mathbb{R}^3$  that interchange the coordinate axes because  $\varphi_{\pi}^* \mathring{e}^i = \mathring{e}^{\pi(i)}$ , which generally differs from  $\mathring{e}^i$ . Thus, whereas the definition (8) of the coordinates  $(c^i, p_i)$  presumes that  $A^x \propto \mathrm{d}x$ ,  $A^y \propto \mathrm{d}y$ , and so forth, the pullback  $\varphi_{\pi}^* A_a^i$  no longer necessarily satisfies this parallelism condition. This difficulty is easy to fix, however, by incorporating an appropriate, internal gauge rotation  $R \in SO(3)$  such that

$$\varphi_{(\pi,R)}:{}^{\gamma}A_a^i\mapsto{}^{\gamma}\tilde{A}_a^i:=\sum_{i}R^i{}_{j}\,\varphi_{\pi}^{*\,\gamma}A_a^j=\sum_{i}R^i{}_{j}\,c^j\,\frac{\mathring{e}_a^{\pi(j)}}{L_j}$$

is again proportional to  $\mathring{e}_a^i$ , and similarly for the physical (co-)triad  $e_a^i$ . The rotation here must be chosen such that  $R^i{}_j = 0$  unless  $\pi(j) = i$ . The set of rotations mapping the coordinate axes into one another like this form the (chiral) octahedral group  $O \subset SO(3)$ , i.e. the subgroup of rotations preserving the unit cube. For any fixed  $\pi \in S_3$ , there are exactly four rotations satisfying the above condition, differing from one another by half-rotations about one of the coordinate axes. Choosing any one of them leads to

$$\varphi_{(\pi,R)}:(c^{i},p_{i})\mapsto(\tilde{c}^{i},\tilde{p}_{i}):=\left(m_{i}\,c^{\pi^{-1}(i)},\frac{1}{m_{i}}\,p_{\pi^{-1}(i)}\right)\quad\text{with}\quad m_{i}:=R^{i}_{\pi^{-1}(i)}\,\frac{L_{i}}{L_{\pi^{-1}(i)}}.$$

(Note that  $R^i_{\pi^{-i}(i)} = \pm 1$  and  $|m_x m_y m_z| = 1$  by definition.) Composing with an appropriate scaling transformation from (9) thus leads to a transformation that simply permutes the  $(c^i, p_i)$  coordinates in pairs.

The residual automorphism group  $\operatorname{Aut}_R$  is the set of *distinct* phase-space transformations induced by the restricted diffeomorphisms described above. In detail,  $\operatorname{Aut}_R \cong [\overline{\operatorname{Diff}} \times SO(3)]_{\parallel}/K_{\Gamma}$  is isomorphic to the group of restricted diffeomorphisms, extended to include (homogeneous) internal gauge rotations, then restricted to preserve the parallelism of (8), and finally quotiented by the (normal) subgroup  $K_{\Gamma}$  of such transformations that act as the identity in phase space. The resulting group is naturally a semi-direct product  $\operatorname{Aut}_R = (\operatorname{Dil}_R \times \operatorname{Par}_R) \rtimes \operatorname{Rot}_R$  of three distinct factors, consisting of

(a) Anisotropic dilatations  $\varphi_t \in \text{Dil}_R \cong \mathbb{R}^3_+$ , labeled by  $\mathbf{t} \in \mathbb{R}^3$  and having the form

$$\varphi_{\mathbf{t}}(c^i, p_i) := \left( e^{-t_i} c^i, e^{t_i - T} p_i \right) \quad \text{with} \quad T := \sum_i t_i; \tag{10}$$

(b) Partial reflections  $\varphi_{\zeta} \in \operatorname{Par}_R \cong S_2^3$ , labeled by  $\zeta \in \{\pm 1\}^3$  and having the form

$$\varphi_{\zeta}(c^{i}, p_{i}) := \left(\zeta_{i} c^{i}, \zeta_{i} p_{i}\right); \tag{11}$$

(c) and residual rotations  $\varphi_{\pi} \in \text{Rot}_R \cong S_3$ , labelled by  $\pi \in S_3$  and having the form

$$\varphi_{\pi}(c^i, p_i) := \left(c^{\pi(i)}, p_{\pi(i)}\right). \tag{12}$$

Note that the partial reflections and residual rotations together define a natural action of the (achiral) octahedral group  $\operatorname{Par}_R \rtimes \operatorname{Rot}_R \cong O_h \subset O(3)$ , which is the full isometry group of the unit cube, including reflections. The residual automorphism group has a non-trivial center  $Z(\operatorname{Aut}_R)$ , consisting of

(i.S) Isotropic dilatations  $\varphi_T \in \text{Dil}_S \cong \mathbb{R}_+$ , labeled by  $T \in \mathbb{R}$  and having the form

$$\varphi_T(c^i, p_i) := \left( e^{-T/3} c^i, e^{-2T/3} p_i \right);$$
 (13)

(ii.S) and isotropic reflections  $\varphi_Z \in \operatorname{Par}_S \cong S_2$ , labeled by  $Z \in \{\pm 1\}$  and having the form

$$\varphi_{Z}(c^{i}, p_{i}) := \left(Z c^{i}, Z p_{i}\right). \tag{14}$$

We refer to  $Z(\operatorname{Aut}_R) \lhd \operatorname{Aut}_R$  as the isotropic automorphism group not only because its elements 'act isotropically' in the Bianchi I phase space, but also because it is naturally isomorphic to the group of residual automorphisms analogous to  $\operatorname{Aut}_R$  for the fully reduced, isotropic model to be discussed in the next section. The quotient group  $\operatorname{Aut}_R/Z(\operatorname{Aut}_R)$  plays a pivotal role in relating the Bianchi I model to its isotropic reduction. This quotient can be identified with the (normal) subgroup  $\operatorname{Aut}_R^0 \lhd \operatorname{Aut}_R$  having T=0 in (10) and  $\zeta_x \zeta_y \zeta_z = 1$  in (11). We refer to this as the proper residual automorphism group because its elements preserve both the symplectic structure (7) and the orientation of the physical triad (2).

Turning now to the dynamics of the Bianchi I model, recall that the gravitational part of the classical Hamiltonian constraint involves the curvature of the homogeneous Ashtekar connection (5):

$${}^{\gamma}F_{ab}i := \mathrm{d}^{\gamma}A^{i}_{ab} + \sum_{ik} \epsilon^{i}_{jk} {}^{\gamma}A^{j}_{a} {}^{\gamma}A^{k}_{b} = \frac{L_{i}}{L_{x}L_{y}L_{z}} \frac{c^{x}c^{y}c^{z}}{c^{i}} \sum_{ik} \epsilon^{i}_{jk} \mathring{e}^{j}_{a} \mathring{e}^{k}_{b}. \tag{15}$$

The coordinate scales  $L_i$  enter because the result is expressed in terms of the fiducial triad. One can relate it instead to the physical triad by solving for the original scale factors  $a_i$ :

$$p_{i} = \frac{L_{x}L_{y}L_{z}}{L_{i}} \frac{|a_{x}a_{y}a_{z}|}{a_{i}} \rightsquigarrow a_{i} = \frac{1}{L_{i}} \frac{\text{vol}(\mathbf{p})}{p_{i}} \quad \text{with} \quad \text{vol}(\mathbf{p}) := |p_{x}p_{y}p_{z}|^{1/2}. \quad (16)$$

Geometrically,  $vol(\mathbf{p})$  is the proper volume of the fiducial cell. Substituting into (15) then gives

$${}^{\gamma}F_{ab}i = \frac{c^x c^y c^z}{c^i} \frac{\operatorname{sgn}(p_x p_y p_z)}{p_i} \sum_{ab}{}^i \quad \text{with} \quad \sum_{ab}{}^i := \sum_{ik} \epsilon^i{}_{jk} e^j_a e^k_b. \tag{17}$$

This result can be expressed compactly in terms of the directional Hubble rates

$$\theta_i := \frac{\mathcal{L}_u a_i}{a_i} = \frac{\dot{a}_i}{N a_i} = \frac{c^i p_i}{\gamma \operatorname{vol}(\mathbf{p})} \leadsto {}^{\gamma} A_a^i = \gamma K_a^i = \gamma \theta_i e_a^i. \tag{18}$$

Each Hubble rate is invariant under anisotropic dilatations (10) and partial reflections (11), and they permute covariantly under the residual rotations of (12). Meanwhile, the curvature of (17) is given by

$${}^{\gamma}F_{ab}i = \gamma^2 \frac{\theta_x \theta_y \theta_z}{\theta_i} \, \Sigma_{ab}{}^i = \gamma^2 \sum_{ik} \epsilon^i{}_{jk} \, \theta_j \, \theta_k \, e_a^j \, e_b^k. \tag{19}$$

This yields a compact expression for (the gravitational part of) the Hamiltonian constraint:

$$H_{g}[N] := \frac{1}{2\kappa} \int_{\mathcal{V}} \sum_{ij} \left( \frac{N E_{i}^{a} E_{j}^{b}}{|\det E|^{1/2}} \left( \sum_{k} \epsilon^{ij_{k}} {}^{\gamma} F_{ab}^{k} - 2(1 + \gamma^{2}) K_{[a}^{i} K_{b]}^{j} \right) \right)$$

$$= -\frac{\operatorname{sgn}(\det e)}{\kappa \gamma^{2}} \int_{\mathcal{V}} N \sum_{k} {}^{\gamma} F_{k} \wedge e_{k}$$

$$= -\frac{\operatorname{vol}[N](\mathbf{p})}{\kappa} \sum_{i < j} \theta_{i} \theta_{j}. \tag{20}$$

The two terms in the integrand on the first line are proportional to one another in the homogeneous case because  $d^{\gamma}A_{ab}{}^{i} = 0$ . Meanwhile,  $vol[N](\mathbf{p})$  denotes the lapse N integrated over the fiducial cell using the proper volume element determined by  $\mathbf{p}$ . Note that  $H_g[N]$  is invariant under the same subgroup of residual automorphisms that preserve the symplectic structure (7), and that its Hamiltonian flow preserves the submanifold of homogeneous states in the phase space of the full theory if and only if N is homogeneous.

#### 2.2. Regularization strategy

The curvature (15) has no operator analogue in the Ashtekar–Lewandowski quantization of gravity. One therefore introduces a *regularized* curvature at the classical level for the Bianchi I model [28]. The regularized curvature is constructed from holonomies along finite curves, which do have operator analogues in the full theory. This classical regularization should therefore be viewed as a part of the quantization process.

It is natural in Bianchi I to consider the holonomy around a rectangular loop with edges parallel to two of the three principal curvature axes. Working in the fundamental representation of SU(2), the holonomy of the connection (5) along a line segment of coordinate length  $\ell$  parallel to the  $x^i$ -axis is given by

$$h_i(\ell) = 1 \cos \frac{c^i \ell}{2L_i} + 2\tau_i \sin \frac{c^i \ell}{2L_i},$$

where 1 denotes the  $2 \times 2$  identity matrix, and  $\tau_i$  are the anti-Hermitian generators of the fundamental representation of SU(2), related to the Pauli matrices by  $\sigma_i = 2i\tau_i$ . It follows that the holonomy around a closed, rectangular plaquette with edges of coordinate lengths  $\ell_i$  and  $\ell_i$  parallel to the  $x^i$ - and  $x^j$ -axes, respectively, is

$$\begin{split} h_{ij}(\ell) &\coloneqq h_j(-\ell_j) \, h_i(-\ell_i) \, h_j(\ell_j) \, h_i(\ell_i) \\ &= \left(1 - 2 \sin^2 \frac{c^i \ell_i}{2L_i} \sin^2 \frac{c^j \ell_j}{2L_j} \right) 1 + 2 \sin \frac{c^i \ell_i}{L_i} \sin^2 \frac{c^j \ell_j}{2L_j} \, \tau_i \\ &- 2 \sin^2 \frac{c^i \ell_i}{2L_i} \sin \frac{c^j \ell_j}{L_j} \, \tau_j - \sin \frac{c^i \ell_i}{L_i} \sin \frac{c^j \ell_j}{L_j} \left[\tau_i, \tau_j\right], \end{split}$$

where  $\ell := (\ell_x, \ell_y, \ell_z)$ . The last term here is quadratic as  $\ell \to 0$ , and proportional to the curvature  ${}^{\gamma}F_{ab}k$  from (15) in that limit. More precisely, we have

$$\lim_{\ell \to 0} \sum_{ij} \operatorname{Tr} \left[ h_{ij}(\ell) \, \tau^k \right] \, \frac{\mathring{e}_a^i}{\ell_i} \, \frac{\mathring{e}_b^j}{\ell_j} \to \frac{1}{2} \, {}^{\gamma} F_{ab} k. \tag{21}$$

It is tempting to define the regularized curvature simply by removing the limit. But the continuum curvature  ${}^{\gamma}F_{ab}k$  from (15) has the property that its pull-back to the plane orthogonal to  $e^a_k$  is proportional to  $\tau^k$ , whereas the expression under the limit in (21) does not. Happily, the cubic terms that create this difficulty cancel one another if instead we set

$${}^{\gamma}F_{ab}k(\ell) := \sum_{ij} \operatorname{Tr} \left[ \left( h_{ij}(\ell) + h_{ij}(-\ell) \right) \tau^{k} \right] \frac{\mathring{e}_{a}^{i}}{\ell_{i}} \frac{\mathring{e}_{b}^{j}}{\ell_{j}} = \sum_{ij} \sin \frac{c^{i}\ell_{i}}{L_{i}} \sin \frac{c^{j}\ell_{j}}{L_{j}} \epsilon_{ij}^{k} \frac{\mathring{e}_{a}^{i}}{\ell_{i}} \frac{\mathring{e}_{b}^{j}}{\ell_{j}}. \tag{22}$$

This regularized curvature is amenable to quantization, though again it depends on the unphysical, coordinate lengths of the plaquette edges.

The Bianchi I model is spatially homogeneous, so the proper length  $s_i$  of any line segment along a symmetry axis is proportional to its coordinate length  $\ell_i$ . Accordingly, we may set

$$\ell_i \, \mathring{e}_i^a = s_i \, e_i^a \leadsto \frac{\ell_i}{L_i} = \frac{p_i \, s_i}{\operatorname{vol}(\mathbf{p})}$$

to define a vector  $\ell$  of coordinate edge lengths corresponding to a given vector  $\mathbf{s}$  of proper edge lengths. The holonomy along an edge of fixed proper length is denoted

$$\bar{h}_i(s) = 1 \cos \frac{c^i p_i s}{2 \operatorname{vol}(\mathbf{p})} + 2\tau_i \sin \frac{c^i p_i s}{2 \operatorname{vol}(\mathbf{p})}.$$
 (23)

Recasting the regularized curvature (22) in terms of proper lengths gives

$${}^{\gamma}\bar{F}_{ab}k(\mathbf{S}) := \sum_{ij} \operatorname{Tr}\left[\left(\bar{h}_{ij}(\mathbf{S}) + \bar{h}_{ij}(-\mathbf{S})\right) \tau^{k}\right] \frac{e_{a}^{i}}{s_{i}} \frac{e_{b}^{j}}{s_{j}} = \sum_{ij} \sin \frac{c^{i}p_{i}s_{i}}{\operatorname{vol}(\mathbf{p})} \sin \frac{c^{j}p_{j}s_{j}}{\operatorname{vol}(\mathbf{p})} \epsilon_{ij}^{k} \frac{e_{a}^{i}}{s_{i}} \frac{e_{b}^{j}}{s_{j}}.$$

$$(24)$$

This expression coincides, for appropriate choices of the  $s_i$  to be described in the next subsection, with the regularized curvature obtained in [27, 28], though the latter is written in terms of its components relative to the *fiducial* triad basis. Comparing with (19), the present expression suggests defining a regularized version of the directional Hubble rate by setting

$$\bar{\theta}_i(s) := \frac{1}{\gamma s} \sin \frac{c^i p_i s}{\text{vol}(\mathbf{p})}.$$
 (25)

Note that, like the ordinary directional Hubble rates (18), these expressions are invariant under anisotropic dilatations (10) and partial reflections (11), and permute covariantly under residual rotations (12).

The standard construction of the Hamiltonian constraint in full LQG, due to Thiemann [30], begins by observing that

$$e_c^k(x) = \frac{2}{\kappa \gamma} \frac{\left\{ A_c^k(x), \text{vol}[N] \right\}}{N(x)}.$$

The connection in the Poisson bracket can be regularized in terms of holonomies by noting that, for an arbitrary curve  $\xi(t)$ , one has

$$\dot{\xi}^{c}(0) \left\{ {}^{\gamma}A_{c}^{k}\left(\xi(0)\right), \text{vol}[N] \right\} = -2 \text{ Tr} \left[ \tau^{k} \frac{\mathrm{d}}{\mathrm{d}t} \left( h_{\xi}^{-1}(t) \left\{ h_{\xi}(t), \text{vol}[N] \right\} \right)_{t=0} \right].$$

We take  $\xi(t)$  to run along one of the principal axes in the Bianchi I case, and parameterize the curve by proper length. Approximating the derivative with a finite difference then leads to

$$\left\{{}^{\gamma}\bar{A}_c^k, \operatorname{vol}[N](\mathbf{p})\right\}(\mathbf{s}) \coloneqq -2\sum_{l}\frac{e_c^l}{s_l}\operatorname{Tr}\left[\tau^k\,\bar{h}_l(-\mathbf{s})\,\left\{\bar{h}_l(\mathbf{s}), \operatorname{vol}[N](\mathbf{p})\right\}\right].$$

Substituting this result and the regularized curvature (24) into the Hamiltonian constraint from the second line of (20) gives the regularized Hamiltonian constraint

$$H_{g}[N](\mathbf{s}) = -\frac{\text{vol}[N](\mathbf{p})}{\kappa^{2}\gamma^{3}} \sum_{ijk} \frac{\epsilon_{ijk}}{s_{i}s_{j}s_{k}} \operatorname{Tr}\left[\left(\bar{h}_{ij}(\mathbf{s}) + \bar{h}_{ij}(-\mathbf{s})\right) \bar{h}_{k}(-\mathbf{s}) \left\{\bar{h}_{k}(\mathbf{s}), \operatorname{vol}(\mathbf{p})\right\}\right], \quad (26)$$

where we have used the identity

$$\sum_{k} \operatorname{Tr}(X\tau^{k}) \operatorname{Tr}(Y\tau_{k}) = \frac{\operatorname{Tr}(X) \operatorname{Tr}(Y) - 2 \operatorname{Tr}(XY)}{4}.$$

To compare this result to the expression from [27, 28], one can explicitly calculate the Poisson bracket

$$\{\bar{h}_k(s), \operatorname{vol}(\mathbf{p})\} = \frac{\kappa \gamma s}{2} \tau_k \, \bar{h}_k(s).$$

Since  $\tau_k$  commutes with  $\bar{h}_k(s)$ , the trace in (26) reduces to the same one from (24), yielding

$$H_{g}[N](\mathbf{s}) = -\frac{\operatorname{vol}[N](\mathbf{p})}{\kappa} \sum_{i < j} \left( \frac{1}{\gamma s_{i}} \sin \frac{c^{i} p_{i} s_{i}}{\operatorname{vol}(\mathbf{p})} \right) \left( \frac{1}{\gamma s_{j}} \sin \frac{c^{j} p_{j} s_{j}}{\operatorname{vol}(\mathbf{p})} \right). \tag{27}$$

Thus, the regularized Hamiltonian constraint has exactly the form of the last expression from (20), but with the directional Hubble rates  $\theta_i$  replaced by their regularized analogues  $\bar{\theta}_i(\mathbf{s})$  from (25). Once again this expression coincides, for appropriate choices of the  $s_i$ , with the Hamiltonian constraint from [27, 28]. (Note that the latter is presented only in the harmonic time gauge, where the lapse  $N = N_0 \operatorname{vol}(\mathbf{p})$  is spatially constant, but state-dependent.)

#### 2.3. Quantum theory

Quantizing the regularized expressions from the previous subsection entails promoting holonomies to quantum operators, and specifying operator orderings where ambiguities arise. To quantize the holonomies (23), Ashtekar and Wilson-Ewing define the complex exponentials

$$\Delta_i(s) := \exp{-\frac{\mathrm{i}c^i|p_i|s}{2\operatorname{vol}(\mathbf{p})}}$$
 (28)

at the classical level. Note the absolute value  $|p_i|$  in the numerator here, which renders  $\Delta_i(s)$  invariant under anisotropic dilatations (10), but *not* under partial reflections (11). Instead, we have  $\varphi_{\zeta}^*\Delta_i(s) = \Delta_i(\zeta_i s)$ . This seemingly undesirable asymmetry is critical for quantization, as we now show.

One *motivates* the quantization of the functions (28) by recalling that the classical coordinate  $c^i$  becomes a derivative operator in a Schrödinger representation based on **p**:

$$c^{i} \mapsto i\hbar\kappa\gamma \frac{\partial}{\partial p_{i}} \longrightarrow -\frac{i|p_{i}|c^{i}s}{2\operatorname{vol}(\mathbf{p})} \mapsto \frac{\hbar\kappa\gamma |p_{i}|^{1/2}s}{2|p_{x}p_{y}p_{z}|^{1/2}} \cdot |p_{i}|^{1/2} \frac{\partial}{\partial p_{i}}.$$
 (29)

The first factor on the right is independent of  $p_i$ , and thus can be treated as a constant along each orbit of this vector field on  $\mathbb{R}^3$ . The second factor can be affinely parameterized such that

$$|p_i|^{1/2} \frac{\partial}{\partial p_i} = \frac{|p_0|^{1/2}}{2p_0} \frac{\partial}{\partial \lambda_i} \quad \text{with} \quad p_i =: p_0 P(\lambda_i) := p_0 \operatorname{sgn}(\lambda_i) \lambda_i^2, \tag{30}$$

where  $p_0$  is an arbitrary constant with units of area to be fixed below. The resulting affine parameter  $\lambda_i$  is dimensionless and increases (as long as  $p_0 > 0$ ) monotonically with  $p_i$ . Thus, a Schrödinger representation based on  $\mathbf{p}$  is closely related to a Schrödinger representation based on  $\lambda$ , though the two have different natural inner products since  $\mathrm{d}^3 p = |p_0|^{3/2} \operatorname{vol}(\mathbf{p}) \, \mathrm{d}^3 \lambda$ . More importantly, however, the vector field in question is a constant multiple of  $\frac{\partial}{\partial \lambda_i}$  on each of its integral curves, and therefore generates a rigid translation in  $\lambda_i$ . It follows that the natural (Schrödinger) quantization of  $\Delta_i(s)$  is such that

$$\langle \lambda | \, \hat{\Delta}_i(s) := \left\langle \lambda + \frac{\hbar \kappa \gamma s_0}{4 p_0 |p_0|^{1/2}} \frac{|\lambda_i|}{|\lambda_x \lambda_y \lambda_z|} \frac{s}{s_0} \, \mathbf{e}_i \right|,\tag{31}$$

where  $\mathbf{e}_i$  is the canonical basis vector in  $\mathbb{R}^3$  and  $s_0$  is a length scale to be fixed below. As usual, the dual basis vectors  $\langle \lambda |$  here map a state  $|\psi\rangle$  to its value  $\psi(\lambda)$  at a particular point  $\lambda \in \mathbb{R}^3$ . Note that, if we were to replace  $|p_i|$  with  $p_i$  on the right side of (28), then the flow of this vector field would reverse in the half-space  $\lambda_i < 0$ , and therefore would not be *globally* integrable [27]. (For s < 0, for example, the flow would converge on the plane  $\lambda_i = 0$  from

both sides in finite affine parameter 'time,' and one cannot continue to integrate through that plane.)

Although the Schrödinger representation based on **p** motivates the quantization (31) of  $\Delta_i(s)$ , the resulting operator needs to act in the 'polymer' Hilbert space [28] of LQC. The inner product on this space is the *sum* 

$$\langle \phi, \psi \rangle = \sum_{\mathbf{p}} \bar{\phi}(\mathbf{p}) \, \psi(\mathbf{p}) = \sum_{\lambda} \bar{\phi}(\lambda) \, \psi(\lambda).$$
 (32)

The distinction is important. The ordering  $|p_i|^{1/2} c^i \mapsto |\hat{p}_i|^{1/2} \hat{c}^i$  chosen in (29) is the unique one that leaves a *constant* wave function  $\psi(\mathbf{p}) = \psi_0$  invariant under the action of the resulting translation operator. But this ordering is not Hermitian in the Schrödinger representation based on  $\mathbf{p}$ , and its exponential  $\hat{\Delta}_i(s)$  is not unitary: this is because the Lebesgue measure  $d^3 p$  is not invariant under a rigid translation in  $\lambda$ . The polymer representations based on  $\mathbf{p}$  and  $\lambda$  are the same, however, so (31) is unitary in LQC.

Typically one would take the limit  $s \to 0$  after quantization to remove the regulator in (31), but that limit does not exist in LQC. Instead, one fixes a certain *finite* value of **s** to define *the* curvature and Hamiltonian constraint operators by setting

$$s_0^2 := \hbar \kappa |\gamma| \sqrt{j_0(j_0 + 1)},\tag{33}$$

where it is natural to take  $j_0 = \frac{1}{2}$  so that  $s_0^2$  is the minimal quantum of area in full LQG. This fixes the length scale introduced in (31). Then one chooses the area scale  $p_0$  from (30) such that the ratio of dimensional factors in (31) is one half:

$$p_0 = \frac{\hbar \kappa \gamma}{2} \sqrt[6]{4j_0(j_0 + 1)}. (34)$$

With these choices, the basic operators of LQC act according to

$$\langle \lambda | \hat{\Delta}_{i}(s) := \left\langle \lambda + \frac{|\lambda_{i}|}{|\lambda_{x}\lambda_{y}\lambda_{z}|} \frac{s}{2s_{0}} \mathbf{e}_{i} \right| \quad \text{and} \quad \langle \lambda | \hat{p}_{i} := p_{0} P(\lambda_{i}) \langle \lambda |,$$
 (35)

where again  $P(\lambda_i) := \operatorname{sgn}(\lambda_i) \lambda_i^2$ . The regularization scheme for the Hamiltonian constraint in [27, 28], which we extend here to other operators that are needed to enforce the quantum symmetry conditions, simply sets all  $s_i = s_0$ . Accordingly, we introduce the shorthands

$$\hat{\Delta}_{i} := \hat{\Delta}_{i}(s_{0}) \leadsto \langle \lambda | \, \hat{\Delta}_{i} := \left\langle \lambda + \frac{|\lambda_{i}|}{2|\Lambda|} \, \mathbf{e}_{i} \right| \quad \text{with } \Lambda := \lambda_{x} \lambda_{y} \lambda_{z}. \tag{36}$$

For purposes of comparison, the basic holonomy operators  $\hat{E}_i^{\pm}$  from [27]<sup>5</sup> correspond to  $\hat{\Delta}_i^{\pm 2}$  in the notation we use here. Note that the effect of  $\hat{\Delta}_i^{\pm 2}$  is to shift only the  $\lambda_i$  component of the argument of the given wave function  $\psi(\lambda) := \langle \lambda | \psi \rangle$  such that  $\Lambda \mapsto \Lambda^{\pm} := \Lambda \pm \operatorname{sgn}(\Lambda \lambda_i)$ .

The standard approach in LQC is to reduce the regularized Hamiltonian constraint (26) to the scalar form (27) *prior* to quantization. To do this, write (27) in the form

$$H_{\mathbf{g}}[N](\mathbf{s}) = -\frac{\operatorname{vol}[N](\mathbf{p})}{\kappa} \sum_{i < j} \left( \frac{\operatorname{sgn} \ p_{i}}{\gamma s_{i}} \frac{\Delta_{i}(2s_{i}) - \Delta_{i}(-2s_{i})}{2i} \right) \left( \frac{\operatorname{sgn} \ p_{j}}{\gamma s_{j}} \frac{\Delta_{j}(2s_{j}) - \Delta_{j}(-2s_{j})}{2i} \right). \tag{37}$$

<sup>&</sup>lt;sup>5</sup> The same notation,  $\hat{E}_i^-$ , is used in [28] to denote a slightly different operator, which omits the absolute value in the denominator from (36). That operator is not unitary, however. See [27] for a corrected expression.

The operator analogues of the various factors in this expression do not commute, and one must choose how to order them in defining the operator analogue of the Hamiltonian constraint. Ashtekar and Wilson-Ewing [28] first choose a Weyl ordering for each factor in braces, the directional Hubble rates from (25), defining the corresponding operators<sup>6</sup>

$$\hat{\theta}_{i}(s_{i}) := \frac{\operatorname{sgn} \hat{\lambda}_{i} (\hat{\Delta}_{i}(-2s_{i}) - \hat{\Delta}_{i}(2s_{i})) + (\hat{\Delta}_{i}(-2s_{i}) - \hat{\Delta}_{i}(2s_{i})) \operatorname{sgn} \hat{\lambda}_{i}}{4i\gamma s_{i}} 
= \left(\hat{\Delta}_{i}(-2s_{i}) \Theta\left(|\hat{\Lambda}| + (s_{i}/s_{0}) \operatorname{sgn} \hat{\lambda}_{i}\right) - \hat{\Delta}_{i}(2s_{i}) \Theta\left(|\hat{\Lambda}| - (s_{i}/s_{0}) \operatorname{sgn} \hat{\lambda}_{i}\right)\right) \frac{\operatorname{sgn} \hat{\lambda}_{i}}{2i\gamma s_{i}} 
= \frac{\operatorname{sgn} \hat{\lambda}_{i}}{2i\gamma s_{i}} \left(\Theta\left(|\hat{\Lambda}| - (s_{i}/s_{0}) \operatorname{sgn} \hat{\lambda}_{i}\right) \hat{\Delta}_{i}(-2s_{i}) - \Theta\left(|\hat{\Lambda}| + (s_{i}/s_{0}) \operatorname{sgn} \hat{\lambda}_{i}\right) \hat{\Delta}_{i}(2s_{i})\right),$$
(38)

where  $\Theta(t)$  denotes the Heaviside step function. Setting  $s_i := s_0$  for all i = x, y, z, these become

$$\hat{\theta}_i = \frac{\operatorname{sgn} \hat{\lambda}_i}{2i\gamma s_0} \left( \Theta\left( |\hat{\Lambda}| - \operatorname{sgn} \hat{\lambda}_i \right) \hat{\Delta}_i^{-2} - \Theta\left( |\hat{\Lambda}| + \operatorname{sgn} \hat{\lambda}_i \right) \hat{\Delta}_i^{+2} \right). \tag{39}$$

Ashtekar and Wilson-Ewing then distribute the volume factor from outside the sum in (20) and (37) symmetrically and again choose a Weyl ordering for the product  $\theta_i \theta_j$  to write

$$\hat{H}_{g} = -\frac{1}{2\kappa} \sum_{i \neq j} |\hat{v}|^{\frac{1+n}{4}} \,\hat{\theta}_{i} \,|\hat{v}|^{\frac{1+n}{2}} \,\hat{\theta}_{j} \,|\hat{v}|^{\frac{1+n}{4}},\tag{40}$$

where  $\langle \lambda | \hat{v} := v_0 \Lambda \langle \lambda |$  denotes the *signed* volume operator and  $v_0 := |p_0|^{3/2}$  is the natural quantum of volume. This expression uses a state-dependent lapse N proportional to the nth power of the volume. The harmonic time gauge used in [28] corresponds to n = 1.

#### 3. Reduction to the isotropic model

#### 3.1. Reduction of the symmetry constraints

The companion paper [15] selects the homogeneous and isotropic section of general relativity by setting

$$\mathbb{S}[f,g] := \mathbb{B}[f] \operatorname{vol}[g] - \operatorname{vol}[f] \mathbb{B}[g] \approx 0, \tag{41}$$

for arbitrary smearing fields  $f_{ij}$  and  $g_{ij}$ , where

$$\mathbb{B}[f] := \operatorname{sgn}(\det e) \sum_{i} \int_{\mathcal{V}} \mathbb{F}^{i} \wedge e^{j} f_{ij} \quad \text{and} \quad \operatorname{vol}[f] := \int_{\mathcal{V}} \operatorname{tr} f |\det e|. \tag{42}$$

<sup>&</sup>lt;sup>6</sup> The present notation suggests a simpler ordering, namely  $\hat{\theta}_i = (\hat{\Delta}_i(-s) \operatorname{sgn} \hat{\lambda}_i \hat{\Delta}_i(-s) - \hat{\Delta}_i(s) \operatorname{sgn} \hat{\lambda}_i \hat{\Delta}_i(s))/2i\gamma s$ . However, the choice of ordering does not matter in the limit of large fiducial cell volume (removal of the infrared regulator) usually used to extract physical predictions [11, 24], whence we retain the conventional ordering of [28]. 
<sup>7</sup> Even classically one has  $\{\theta_i, \theta_j\} = \kappa (\theta_i - \theta_j)/2 \operatorname{vol}(\mathbf{p})$ , so some ordering prescription for the directional Hubble factors is required.

The curvature appearing in the definition of  $\mathbb{B}[f]$  is that of the complexified connection

$$\mathbb{A}_a^i := A_a^i + i\alpha \, e_a^i,\tag{43}$$

where  $\alpha$  is an arbitrary, but fixed, real constant with units of inverse length. The conditions (41) imposing homogeneity and isotropy in this approach are diffeomorphism covariant in the sense that replacing both the fundamental fields (A, E) and the smearing fields (f, g) with their images under a spatial diffeomorphism leaves  $\mathbb{S}[f, g]$  unchanged. Requiring (41) for *all* choices of the smearing fields therefore selects those points (A, E) of the phase space that are invariant under *some* action, as opposed to under a *fixed* action, of one of the symmetry groups appropriate for isotropic and homogeneous cosmologies.

The symmetry conditions (41) simplify considerably when restricted to the phase space of Bianchi I cosmologies described in the previous section. Specifically, (43) becomes

$$\mathbb{A}^i = \mathbb{C}^i \frac{\mathring{e}^i}{L_i} := \left( c^i + i\alpha \frac{\operatorname{vol}(\mathbf{p})}{p_i} \right) \frac{\mathring{e}^i}{L_i},$$

and the functionals from (42) become

$$\mathbb{B}[f] = \sum_{i} \frac{p_x \, p_y \, p_z \, \mathbb{c}^x \, \mathbb{c}^y \, \mathbb{c}^z}{p_i \, \mathbb{c}^i \, \text{vol}^2(\mathbf{p})} \int_{\mathcal{V}} f_{ii} \, |\text{det } e| \quad \text{and} \quad \text{vol}[f] = \sum_{i} \int_{\mathcal{V}} f_{ii} \, |\text{det } e|,$$

respectively. These both depend on the smearing field  $f_{ij}$  only through the average values

$$f_i := \frac{1}{\operatorname{vol}(\mathbf{p})} \int_{\mathcal{V}} f_{ii} |\det e|$$

of its diagonal components over the fiducial cell. Note that such an average is independent of the (homogeneous) triad field in a Bianchi I geometry. Using these averages, together with the definition (18) of the directional Hubble rates as functions on phase space, then gives

$$\mathbb{B}[f] = \sum_{i} f_{i} \mathbb{B}^{i} := \text{vol}(\mathbf{p}) \sum_{i} f_{i} \left( \prod_{j \neq i} (\gamma \theta_{j} + i\alpha) \right) \quad \text{and} \quad \text{vol}[f] = \text{vol}(\mathbf{p}) \sum_{i} f_{i}. \quad (44)$$

Finally, substituting these expressions into (41) gives the symmetry conditions

$$\mathbb{S}[f,g] = \text{vol}(\mathbf{p}) \sum_{ij} f_i g_j (\mathbb{B}^i - \mathbb{B}^j) \approx 0$$
(45)

that select the isotropic sector of the Bianchi I model.

The content of the reduced symmetry conditions becomes clearer if we rewrite  $\mathbb{B}^i - \mathbb{B}^j = \mathbb{B}^i \, \varsigma^j - \varsigma^i \, \mathbb{B}^j$  in the sum, where  $\varsigma^i$  denotes the vector with all components equal to one. Doing so shows that the symmetry conditions hold for all smearing fields if and only if  $\mathbb{B} \wedge \varsigma = 0$ , meaning that the two vectors are proportional, and thus that  $\mathbb{B}^x = \mathbb{B}^y = \mathbb{B}^z$ . Furthermore, we have that

$$(\gamma \theta_{y} + i\alpha)(\gamma \theta_{z} + i\alpha) = (\gamma \theta_{x} + i\alpha)(\gamma \theta_{z} + i\alpha) = (\gamma \theta_{y} + i\alpha)(\gamma \theta_{z} + i\alpha)$$

$$\Leftrightarrow \theta_{x} = \theta_{y} = \theta_{z}.$$
(46)

Thus, the full content of the symmetry conditions (41) in the Bianchi I model is just that all three directional Hubble rates are the same.

In order to impose the symmetry conditions (45) simultaneously in the canonical formalism, one must check that their Poisson algebra closes. To do so, first define

$$\mathbb{S}[f,g] = \sum_{ijk} \epsilon^{ijk} f_i g_j \mathbb{S}_k \quad \text{with} \quad \mathbb{S}_k := \text{vol}(\mathbf{p}) \sum_{lm} \epsilon_{klm} \, \mathbb{B}^l. \tag{47}$$

The symmetry conditions, for all smearing fields  $f_{ij}$  and  $g_{ij}$ , is equivalent to  $\mathbb{S}_x = \mathbb{S}_y = \mathbb{S}_z = 0$  due to the homogeneity of the Bianchi I model. Furthermore,

$$\begin{aligned}
\{\mathbb{S}_{x}, \mathbb{S}_{y}\} &= \left\{ (c^{x} p_{x} + i\alpha \operatorname{vol}(\mathbf{p})) \left( c^{y} p_{y} - c^{z} p_{z} \right), \left( c^{y} p_{y} + i\alpha \operatorname{vol}(\mathbf{p}) \right) (c^{z} p_{z} - c^{x} p_{x}) \right. \\
&= \left. (c^{x} p_{x} + i\alpha \operatorname{vol}(\mathbf{p})) \left( c^{z} p_{z} - c^{x} p_{x} \right) \left\{ c^{y} p_{y} - c^{z} p_{z}, i\alpha \operatorname{vol}(\mathbf{p}) \right\} \\
&+ \left. \left( c^{y} p_{y} + i\alpha \operatorname{vol}(\mathbf{p}) \right) \left( c^{y} p_{y} - c^{z} p_{z} \right) \left\{ i\alpha \operatorname{vol}(\mathbf{p}), c^{z} p_{z} - c^{x} p_{x} \right\} \\
&+ \left( c^{y} p_{y} - c^{z} p_{z} \right) \left( c^{z} p_{z} - c^{x} p_{x} \right) \left( \left\{ c^{x} p_{x}, i\alpha \operatorname{vol}(\mathbf{p}) \right\} \left\{ i\alpha \operatorname{vol}(\mathbf{p}), c^{y} p_{y} \right) \right\} = 0,
\end{aligned} \tag{48}$$

and cyclic permutations. We have used  $\{c^ip_i,c^jp_j\}=0$  in passing to the second line here, as well as  $\{c^ip_i,\operatorname{vol}(\mathbf{p})\}=\frac{1}{2}\kappa\gamma\operatorname{vol}(\mathbf{p})$  in the final step. This is a stronger result than in the full theory [15], where the Poisson algebra of the symmetry conditions is closed (i.e. the Poisson bracket of two  $\mathbb{S}'s$  is a sum of terms proportional to  $\mathbb{S}'s$ ) but not trivial. A similar calculation shows that

$$\left\{ \mathbb{S}_{x}, \bar{\mathbb{S}}_{y} \right\} = -\mathrm{i}\alpha\kappa\gamma \left( c^{y}p_{y} - c^{z}p_{z} \right) \left( c^{z}p_{z} - c^{x}p_{x} \right) \mathrm{vol}(\mathbf{p}). \tag{49}$$

Although this Poisson bracket does not vanish everywhere in phase space, it does vanish when the symmetry conditions hold. Again, this is a stronger result than in the full theory [15], where the Poisson brackets of the symmetry conditions and their complex conjugates generally do not vanish even weakly, i.e. on the submanifold where the symmetry conditions hold. This result is attributable to the proportionality between each symmetry condition and its complex conjugate in the homogeneous Bianchi I model with coefficient non-zero and smooth throughout  $\Gamma$ ,

$$\bar{\mathbb{S}}_{y} = \left(c^{y} p_{y} - i\alpha \operatorname{vol}(\mathbf{p})\right) \left(c^{z} p_{z} - c^{x} p_{x}\right) = \frac{c^{y} p_{y} - i\alpha \operatorname{vol}(\mathbf{p})}{c^{y} p_{y} + i\alpha \operatorname{vol}(\mathbf{p})} \, \mathbb{S}_{y} =: \eta_{y} \mathbb{S}_{y}, \tag{50}$$

as it implies immediately

$$\{\mathbb{S}_x, \bar{\mathbb{S}}_y\} = \{\mathbb{S}_x, \eta_y\} \mathbb{S}_y + \{\mathbb{S}_x, \mathbb{S}_y\} \eta_y \approx 0.$$
 (51)

#### 3.2. Reduction to the classical isotropic sector

Recall  $\Gamma \cong \mathbb{R}^3 \times \mathbb{R}^3_{\times}$  denotes the classical phase space of the Bianchi I model constructed in the previous section. Let  $\bar{\Gamma} \subset \Gamma$  denote the classical isotropic sector on which the symmetry conditions (41) hold, or equivalently, on which  $\theta_x = \theta_y = \theta_z$ . There are only two independent conditions here, so  $\bar{\Gamma}$  is (locally) a four-dimensional submanifold of the six-dimensional phase space  $\Gamma$ . We can pull the symplectic structure (7) back to  $\bar{\Gamma}$  by first writing

$$\Omega = \frac{1}{\kappa \gamma} \sum_{i} dc^{i} \wedge dp_{i} = \frac{1}{\kappa} \sum_{i} d\left(\frac{\theta_{i} \operatorname{vol}(\mathbf{p})}{p_{i}}\right) \wedge dp_{i} = \frac{1}{\kappa} d\left(\operatorname{vol}(\mathbf{p}) \sum_{i} \theta_{i} d \ln |p_{i}|\right)$$

in complete generality. If we now set  $\theta_x = \theta_y = \theta_z =: \theta$ , then

d ln vol(
$$\mathbf{p}$$
) =  $\frac{1}{2} \sum_{i} d \ln |p_{i}| \quad \rightsquigarrow \quad \underline{\Omega} = \frac{2}{\kappa} d\theta \wedge \underline{d\text{vol}(\mathbf{p})}.$  (52)

This is clearly degenerate, with a kernel consisting of vectors tangent to  $\bar{\Gamma} \subset \Gamma$  that change neither the common value  $\theta$  of the directional Hubble rates, nor the proper volume vol( $\mathbf{p}$ ) of the fiducial cell.

The appropriate, non-degenerate isotropic phase space is the quotient manifold  $\Gamma_S \cong \mathbb{R} \times \mathbb{R}_{\times}$ , consisting of equivalence classes of points  $(c^i, p_i) \in \bar{\Gamma}$  on which the geometric means

$$c := \sqrt[3]{c^x c^y c^z}$$
 and  $p := \sqrt[3]{p_x p_y p_z}$ 

both take constant values. It is sometimes convenient to use the signed volume

$$v := \text{sgn } p |p|^{3/2}$$

instead of p itself as a phase-space coordinate for the isotropic model. The volume and Hubble rate(s) are

$$\underline{\operatorname{vol}(\mathbf{p})} = |p|^{3/2} = |v| \quad \text{and} \quad \theta = \sqrt[3]{\underline{\theta}_x \underline{\theta}_y \underline{\theta}_z} = \frac{c \operatorname{sgn} p}{\gamma |p|^{1/2}} = \frac{c}{\gamma v^{1/3}}$$
 (53)

respectively, on each equivalence class in  $\Gamma_S$ . They therefore descend to well-defined functions on the reduced phase space. Any function of these quantities likewise descends to  $\Gamma_S$ , including in particular the gravitational part (20) of the Hamiltonian constraint

$$\underline{H_g} = -\frac{3}{\kappa \gamma^2} |p|^{(3n+1)/2} c^2 = -\frac{3}{\kappa \gamma^2} |v|^{n+1/3} c^2, \tag{54}$$

where we have fixed the lapse  $N = \text{vol}(\mathbf{p})^n$ , as well as the regularized Hubble rates (25)

$$\underline{\bar{\theta}_i(s)} = \frac{\operatorname{sgn} p}{\gamma s} \sin \frac{cs}{|p|^{1/2}} = \frac{1}{\gamma s} \sin \frac{cs}{v^{1/3}},$$

and the regularized Hamiltonian constraint (27) derived from them. The symplectic structure (52) becomes

$$\underline{\Omega} = \frac{3}{\kappa \gamma} \, \mathrm{d} c \wedge \mathrm{d} p = \frac{2}{\kappa \gamma \, |v|^{1/3}} \, \mathrm{d} c \wedge \mathrm{d} v = \frac{2}{\kappa} \, \mathrm{d} (\theta \, \operatorname{sgn} \, p) \wedge \mathrm{d} v.$$

This clearly descends to  $\Gamma_S$  as well, where it is equivalent to the standard Poisson bracket  $\{c, p\} = \frac{1}{3}\kappa\gamma$  of isotropic LQC.

As mentioned in the previous section, the residual automorphism group for the isotropic model is naturally isomorphic to the center  $Z(Aut_R)$  of the residual automorphism group for the Bianchi I model. In detail, the isotropic dilatations (13) and isotropic reflections (14) act on  $\Gamma_S$  via

$$\varphi_T: (c, p) \mapsto \left( e^{-T/3} c, e^{-2T/3} p \right) \quad \text{and} \quad \varphi_Z: (c, p) \mapsto (Zc, Zp),$$
 (55)

respectively. More importantly, however, the complementary subgroup  $\operatorname{Aut}_R^0 \cong \operatorname{Aut}_R/Z(\operatorname{Aut}_R)$  of proper residual automorphisms acts *transitively* on the equivalence

class of points  $(c^i, p_i) \in \bar{\Gamma}$  corresponding to any given point  $(c, p) \in \Gamma_S$  of the isotropic phase space. To see this, first observe that

$$(c^{i}, p_{i}) = \left(\frac{cp}{\theta} \frac{\theta_{i}}{p_{i}}, \frac{p_{i}}{p} p\right) = \varphi_{t} \circ \varphi_{\zeta} \left(\frac{c}{\theta} \theta_{i}, (p, p, p)\right) \quad \text{with } \begin{cases} t_{i} := \ln|p_{i}| - \ln|p| \\ \zeta_{i} := \operatorname{sgn}(pp_{i}) \end{cases}$$

for any point  $(c^i,p_i)\in\Gamma$ , where  $\theta\coloneqq\sqrt[3]{\theta_x\theta_y\theta_z}$  denotes the geometric mean of the directional Hubble rates. The residual automorphism on the right here is proper because  $\sum_i t_i=0$  and  $\zeta_x\zeta_y\zeta_z=1$  by construction. Inverting it shows that every  $(c^i,p_i)\in\Gamma$  can be put in a 'partly diagonal' form with  $p_x=p_y=p_z=p$  by an appropriate proper residual automorphism. Furthermore, the resulting phase-space point is 'fully diagonal' in the sense that  $c^x=c^y=c^z=c$  as well if and only if  $(c^i,p_i)\in\Gamma$  lies in the classical isotropic sector  $\bar{\Gamma}\subset\Gamma$  where  $\theta_x=\theta_y=\theta_z=\theta$ . This fact characterizes the classical isotropic sector  $\bar{\Gamma}\subset\Gamma$  purely in terms of the action of the residual automorphism group:

**Theorem 1.** A point  $(c^i, p_i) \in \Gamma$  of the Bianchi I phase space lies in the classical isotropic sector  $\bar{\Gamma} \subset \Gamma$  if and only if there exists a residual automorphism  $\varphi \in \operatorname{Aut}_R$  such that

$$\varphi \circ \varphi_{\pi} \circ \varphi^{-1}(c^{i}, p_{i}) = (c^{i}, p_{i}) \tag{56}$$

for all residual rotations  $\varphi_{\pi} \in \text{Rot}_R$ . One may choose  $\varphi \in \text{Aut}_R^0$  to be proper without loss of generality.

#### 3.3. Quantum isotropy and the isotropic model

Working in the Hilbert space  $\mathcal{H}$  of the Bianchi I model, we define the (regularized) operator analogues of the functions  $\mathbb{S}_i$  from (47) that define the classical isotropic sector as follows:

$$\hat{\mathbb{S}}_{x}(s) = |\hat{v}|^{\frac{1}{2}} \frac{\left(\gamma \hat{\theta}_{x}(s) + i\alpha\right) |\hat{v}| \left(\gamma \hat{\theta}_{z}(s) - \gamma \hat{\theta}_{y}(s)\right) + \left(\gamma \hat{\theta}_{z}(s) - \gamma \hat{\theta}_{y}(s)\right) |\hat{v}| \left(\gamma \hat{\theta}_{x}(s) + i\alpha\right)}{2} |\hat{v}|^{\frac{1}{2}}, (57)$$

and cyclic permutations. The regularized Hubble rate operators  $\hat{\theta}_i(s)$  are defined in (38), and the ordering prescription adopted here at the quantum level mimics that of the Hamiltonian constraint from (40). The quantum isotropic sector is the subspace  $\mathcal{V}_{\text{symm}} \subset \mathcal{H}$  of Bianchi I states that are annihilated by all three operators  $\hat{\mathbb{S}}_i$ . It is not obvious at the moment that any such states exist. But we will see in the next section that indeed they do by showing that all three operators annihilate every state in a particular embedding of the Hilbert space of the fully isotropic theory into  $\mathcal{H}$ .

To compare the isotropic sector of the quantum Bianchi I model to the quantum isotropic model—wherein isotropy is imposed at the classical level, prior to quantization—we must of course review the quantization of the fully reduced model itself. It proceeds [12] similarly to that of the Bianchi I model presented in detail above. We introduce the exponentials

$$\Delta(s) := \exp{-\frac{ic \, s}{2|p|^{1/2}}},$$

and motivate their quantization by recalling that c becomes a differential operator in a Schrödinger quantization based on p, and

$$\hat{\Delta}(s) := \exp \frac{s\hbar\kappa\gamma}{6|p|^{1/2}} \frac{\mathrm{d}}{\mathrm{d}p} = \exp \frac{s\hbar\kappa\gamma}{4} \frac{\mathrm{d}}{\mathrm{d}v}.$$

a shift operator acting on  $\hat{v}$  eigenstates as

$$\langle v|\hat{\Delta}(s) = \left\langle v + \frac{s\hbar\kappa\gamma}{4} \right| = \left\langle v + \frac{1}{2}\frac{s}{s_0}v_0 \right|.$$

The Hubble rate (53) can again be expressed as limits of combinations of  $\Delta(s)$  and v:

$$\theta = \lim_{s \to 0} \theta(s) := \lim_{s \to 0} \frac{\operatorname{sgn} \ v(\Delta(-2s) - \Delta(2s))}{2i\gamma s}.$$

Weyl ordering yields the regulated operator

$$\hat{\theta}(s) = \frac{\operatorname{sgn} \hat{v}(\hat{\Delta}(-2s) - \hat{\Delta}(2s)) + (\hat{\Delta}(-2s) - \hat{\Delta}(2s))\operatorname{sgn} \hat{v}}{4\mathrm{i}\gamma s}$$

$$= \left(\hat{\Delta}(-2s)\Theta\left(|\hat{v}| + (v_0s/s_0)\operatorname{sgn} \hat{v}\right) - \hat{\Delta}(2s)\Theta\left(|\hat{v}| - (v_0s/s_0)\operatorname{sgn} \hat{v}\right)\right) \frac{\operatorname{sgn} \hat{v}}{2\mathrm{i}\gamma s}.$$
(58)

Following [12], we again take the limits to  $s = s_0$ , so that  $\hat{\theta} = \hat{\theta}(s_0)$ . As in the Bianchi I case, the isotropic Hamiltonian constraint (54) can be expressed in terms of v and  $\theta$  and quantized using a symmetric ordering, yielding the constraint operator of [12],

$$\hat{H}_g = -\frac{3}{\kappa} |\hat{v}|^{\frac{1+n}{4}} \hat{\theta} |\hat{v}|^{\frac{1+n}{2}} \hat{\theta} |\hat{v}|^{\frac{1+n}{4}}.$$
 (59)

#### 4. Embedding

#### 4.1. Conditions on, and desired properties of, the embedding

The definition of a gauge- and diffeomorphism-invariant homogeneous isotropic sector in full LQG is only the first part of the strategy outlined in [15]. The second part is to define an embedding  $\iota_{\text{Full}}$  of the isotropic model into this sector, and use this embedding to compare operators and dynamics in the two models. The strategy presented there is to define  $\iota_{\text{Full}}$  by stipulating the following conditions:

- (a)  $\iota_{\text{Full}}$  should map states into the quantum homogeneous isotropic sector. That is, it's image should be annihilated by the symmetry constraint operators  $\hat{\mathbb{S}}[f,g]$  for all f and g.
- (b)  $\iota_{\text{Full}}$  should *intertwine* two pairs of operators  $(\hat{O}_{\text{Full}}^i, \hat{O}_S^i)$ , i = 1, 2 in the full and homogeneous isotropic theories,

$$\hat{O}_{\text{Full}}^{i} \circ \iota_{\text{Full}} = \iota_{\text{Full}} \circ \hat{O}_{S}^{i}, \tag{60}$$

corresponding to the two dimensions of the homogeneous isotropic phase space.

The first condition fixes the image of  $\iota_{\text{Full}}$ , while the second condition fixes how states in this image are identified with states in the homogeneous isotropic model. If we use  $\iota_{\text{Full}}$  to identify homogeneous isotropic states with full theory states, the second condition (60) simply states that  $\hat{O}_{\text{Full}}^i$  should have the same action on homogeneous isotropic states as  $\hat{O}_{\text{S}}^i$ .

For the present paper, the task is to find an embedding  $\iota$  of the isotropic quantum model into the Bianchi I quantum model. The analogue of the above conditions is then

- (a)  $\hat{\mathbb{S}}_i \circ \iota = 0$  for all i.
- (b)  $\hat{O}^i \circ \iota = \iota \circ \hat{O}_S^i$  for two pairs of operators  $(\hat{O}^i, \hat{O}_S^i)$  in the Bianchi I and isotropic models, i = 1, 2.

In contrast to full LQG, in the Bianchi I model there are automorphisms with well-defined action in the quantum theory that are non-trivial *even once the Gauss and diffeomorphism constraints are imposed*. As a consequence, in the Bianchi I case, there is an additional covariance condition which can and must be stipulated:

(c)  $\iota$  should be covariant under all residual automorphisms well-defined in the quantum theory.

As we shall argue below, conditions (a) and (c) are expected to have the same content from classical analysis, and, in the quantum theory, we will see that (c) implies (a). For this reason, we impose (c), and let (a) follow as a consequence<sup>8</sup>. In fact, the classical analysis will lead us to expect not only the equivalence of (a) and (c), but also the equivalence of

$$\overline{(a)}\,\,\hat{\mathbb{S}}_i^{\dagger}\circ\iota=0$$

with both of these, and we will see explicitly in the quantum theory that (c) implies not only (a), but  $\overline{(a)}$  as well.

In this section, our imposition of (c)—basically equivalent to (a)—and (b) will uniquely determine  $\iota$ . This is consistent with the results found for the toy model in appendix B of [15]. Once uniquely determined,  $\iota$  can be used to compare other operators  $(\hat{O}, \hat{O}_s)$  in the two models, again via the intertwining condition

$$\hat{O} \circ \iota_{\text{Full}} = \iota_{\text{Full}} \circ \hat{O}_{S}. \tag{61}$$

Note that if  $\hat{O}_S$  is not known, the above equation will also uniquely determine it. Hence, the above equation can also be thought of as defining a *map* from Bianchi I operators preserving the isotropic sector, to operators in LQC. Remarkably, in the end, we will find that  $\iota$  maps *all* of the physically relevant operators in Bianchi I introduced in section 2.3 exactly to the corresponding operators in the isotropic theory introduced in section 3.3. This includes the Hamiltonian constraint operators in the two models, so that the embedding  $\iota$  will establish that the isotropic model captures both the kinematics and dynamics of the isotropic sector of the quantum Bianchi I *exactly*.

#### 4.2. Unitary action of canonical residual automorphisms

Let  $\mathrm{Dil}_R^o$  denote the *proper anisotropic dilatations*, that is, the dilatations preserving the volume of the fiducial cell. The subgroup of the residual automorphisms introduced in subsection 2.1 that are canonical transformations, hence with unitary action on quantum states, we call the *canonical residual automorphisms*  $\mathrm{Aut}_R^C$ . Explicitly, it is generated by the proper anisotropic dilatations, the partial reflections, and the residual rotations,  $\mathrm{Aut}_R^C = (\mathrm{Dil}_R^o \times \mathrm{Par}_R) \rtimes \mathrm{Rot}_R$ . From equations (10)–(12), for each  $t_x, t_y \in \mathbb{R}$ ,  $\zeta \in \{\pm 1\}^3$ , and  $\pi \in S_3$ , the actions of these three types of transformations in the quantum theory is given by

$$\hat{\varphi}_{(t_x,t_y,-t_x-t_y)}|p_x,p_y,p_z\rangle = |e^{t_x}p_x,e^{t_y}p_y,e^{-t_x-t_y}p_z\rangle,$$

$$\hat{\varphi}_{\zeta}|(p_i)\rangle = |(\zeta_i p_i)\rangle,$$

$$\hat{\varphi}_{\pi}|(p_i)\rangle = |(p_{\pi(i)})\rangle.$$
(62)

<sup>&</sup>lt;sup>8</sup> Once a single superselection sector is picked in the Bianchi I model [28], the implication also goes in the opposite direction. However, the argument for superselection comes from a specific dynamics. Part of the purpose of this work is to test compatibility of the dynamics in the isotropic and Bianchi I models, so that we preferred our presentation to be independent of any one choice of dynamics, and hence independent of any superselection.

As discussed in section 2, the residual automorphisms, when acting on the isotropic phase space, reduce to the group of isotropic automorphisms  $\operatorname{Aut}_S$ . For canonical residual automorphisms  $T := \sum_{i=1}^3 t_i = 0$ , so that  $\operatorname{Aut}_R^C$  reduces to the even smaller group of isotropic reflections  $\operatorname{Par}_S$ . That is, the actions of the proper anisotropic dilatations and residual rotations on the isotropic phase space are trivial, while the action of the partial reflections is given by (55), so that the quantum action is given by

$$\hat{\varphi}_{(t_x,t_y,-t_x-t_y)}|p\rangle = |p\rangle,$$

$$\hat{\varphi}_{\zeta}|p\rangle = |\zeta_1\zeta_2\zeta_3p\rangle,$$

$$\hat{\varphi}_{\pi}|p\rangle = |p\rangle.$$
(63)

#### 4.3. Derivation

Imposition of covariance under residual canonical automorphisms. For the purpose of deriving the embedding, it is convenient to label the momentum basis in Bianchi I using  $\lambda_x$ ,  $\lambda_y$ , and  $\Lambda$  (30), (36), and to label the momentum basis in the isotropic theory also by  $\Lambda$ . In terms of these labels, the action of the most general canonical residual automorphism  $\varphi := \varphi_{(t_x,t_y,-t_x-t_y)} \circ \varphi_\zeta \circ \varphi_\pi$  is given by

$$\hat{\varphi}|\lambda_x,\lambda_y,\Lambda\rangle = |\zeta_x e^{t_x/2} \lambda_{\pi(x)}, \, \zeta_y e^{t_y/2} \lambda_{\pi(y)}, \, \zeta_x \zeta_y \zeta_z \Lambda\rangle$$
$$\hat{\varphi}|\Lambda\rangle = |\zeta_x \zeta_y \zeta_z \Lambda\rangle.$$

Imposing covariance of  $\iota$  under all such transformations,  $\hat{\varphi} \circ \iota = \iota \circ \hat{\varphi}$ , leads to the following condition on the matrix elements of  $\iota$ :

$$\langle \lambda_x, \lambda_y, \Lambda | \iota | \Lambda' \rangle = \langle \zeta_x e^{-t_x/2} \lambda_{\pi(x)}, \zeta_y e^{-t_y/2} \lambda_{\pi(y)}, \zeta_x \zeta_y \zeta_z \Lambda | \iota | \zeta_x \zeta_y \zeta_z \Lambda' \rangle$$
 (64)

for all  $t_x, t_y, \zeta, \pi$ . First setting  $\zeta_z = \zeta_x \zeta_y$  and  $\pi = \mathrm{id}$ , imposing this condition for all  $t_x, t_y, \zeta_x, \zeta_y$  leads to

$$\langle \lambda_x, \lambda_y, \Lambda | \iota | \Lambda' \rangle = \langle \beta_x \lambda_x, \beta_y \lambda_y, \Lambda | \iota | \Lambda' \rangle$$

for all  $\beta_x, \beta_y \in \mathbb{R}_x$ . Since  $\lambda_x \neq 0$  and  $\lambda_y \neq 0$ , setting  $\beta_x = \lambda_x^{-1}$  and  $\beta_y = \lambda_y^{-1}$ , we have

$$\langle \lambda_{r}, \lambda_{v}, \Lambda | \iota | \Lambda' \rangle = \langle 1, 1, \Lambda | \iota | \Lambda' \rangle =: C(\Lambda; \Lambda')$$

for all  $(\lambda_x, \lambda_y, \Lambda) \in \mathbb{R}^3_{\times}$ . These matrix elements then furthermore satisfy (64) for *all* canonical residual automorphisms if and only  $C(\Lambda; \Lambda')$  additionally satisfies  $C(-\Lambda; -\Lambda') = C(\Lambda; \Lambda')$ . Explicitly, the resulting embedding then takes the form

$$\iota|\Lambda'\rangle = \sum_{\lambda_{x},\lambda_{y},\Lambda\neq 0} C(\Lambda;\Lambda')|\lambda_{x},\lambda_{y},\Lambda\rangle = \sum_{\Lambda\neq 0} C(\Lambda;\Lambda') \sum_{\lambda_{x},\lambda_{y}\neq 0} |\lambda_{x},\lambda_{y},\Lambda\rangle =: \sum_{\Lambda\neq 0} C(\Lambda;\Lambda')\iota_{0}|\Lambda\rangle.$$
(65)

Note that, from this condition alone, every non-zero element in the range of  $\iota$  is *necessarily non-normalizable* in the polymer inner product (32). Define  $Cyl_{BI}$  to be the space of finite linear combinations of momentum eigenstates in the Bianchi I Hilbert space. Then, what we are saying is that covariance under canonical residual automorphisms forces the image of  $\iota$  to be represented in the algebraic dual  $Cyl_{BI}^*$ , which includes possibly non-normalizable linear

combinations of momentum eigenstates. This is similar to the kinematical non-normalizability of diffeomorphism-invariant states in the full theory [31].

The image of  $\iota$  then automatically satisfies quantum isotropy independent of ordering ambiguity.

**Lemma 1.**  $\iota_0$  intertwines both  $\hat{v}$  and  $\hat{\theta}_i(s)$  for all s.

**Proof.** That  $\iota_0$  intertwines  $\hat{v}$  is immediate:

$$\iota_0 \circ \hat{v} | \Lambda \rangle = v_0 \Lambda \iota_0 | \Lambda \rangle = v_0 \Lambda \sum_{\lambda_x, \lambda_y \neq 0} | \lambda_x, \lambda_y, \Lambda \rangle = \hat{v} \sum_{\lambda_x, \lambda_y \neq 0} | \lambda_x, \lambda_y, \Lambda \rangle = \hat{v} \circ \iota | \Lambda \rangle.$$

For the  $\hat{\theta}_i(s)$ , it is sufficient to consider  $\hat{\theta}_z(s)$ . Starting from equations (38) and (35), we have for all  $|\Lambda\rangle$ ,

$$\begin{split} \hat{\theta}_{z}(s) \circ \iota_{0} | \Lambda \rangle &= \left[ \Delta_{l}(-2s) \, \Theta \left( \left| \hat{\Lambda} \right| + (s/s_{0}) \, \operatorname{sgn} \, \hat{\lambda}_{z} \right) \right] \frac{\operatorname{sgn} \, \hat{\lambda}_{z}}{2 \mathrm{i} \gamma s} \sum_{\lambda_{x}, \lambda_{y} \neq 0} \left| \lambda_{x}, \lambda_{y}, \Lambda \right\rangle \\ &= \frac{1}{2 \mathrm{i} \gamma s} \sum_{\lambda_{x}, \lambda_{y} \neq 0} \left[ \operatorname{sgn} \left( \frac{\Lambda}{\lambda_{x} \lambda_{y}} \right) \, \Theta \left( \left| \Lambda \right| + (s/s_{0}) \, \operatorname{sgn} \left( \frac{\Lambda}{\lambda_{x} \lambda_{y}} \right) \right) \\ &\times \left| \lambda_{x}, \lambda_{y}, \Lambda + (s/s_{0}) \, \operatorname{sgn}(\lambda_{x} \lambda_{y}) \right\rangle \\ &- \operatorname{sgn} \left( \frac{\Lambda}{\lambda_{x} \lambda_{y}} \right) \, \Theta \left( \left| \Lambda \right| - (s/s_{0}) \, \operatorname{sgn} \left( \frac{\Lambda}{\lambda_{x} \lambda_{y}} \right) \right) \\ &\times \left| \lambda_{x}, \lambda_{y}, \Lambda - (s/s_{0}) \, \operatorname{sgn}(\lambda_{x} \lambda_{y}) \right\rangle \\ &= \frac{\operatorname{sgn} \, \Lambda}{2 \mathrm{i} \gamma s} \sum_{\lambda_{x}, \lambda_{y} \neq 0} \left[ \left\{ \operatorname{sgn} \left( \lambda_{x} \lambda_{y} \right) \, \Theta \left( \left| \Lambda \right| + (s/s_{0}) \right. \right. \\ &\left. \times \left\{ \operatorname{sgn}(\lambda_{x} \lambda_{y}) \right\} \, \operatorname{sgn} \, \Lambda \right) \left| \lambda_{x}, \lambda_{y}, \Lambda + (s/s_{0}) \left\{ \operatorname{sgn}(\lambda_{x} \lambda_{y}) \right\} \right\rangle \\ &+ \left\{ - \operatorname{sgn}(\lambda_{x} \lambda_{y}) \right\} \, \Theta \left( \left| \Lambda \right| + (s/s_{0}) \left\{ - \operatorname{sgn}(\lambda_{x} \lambda_{y}) \right\} \, \operatorname{sgn} \, \Lambda \right) \\ &\times \left| \lambda_{x} \lambda_{y}, \Lambda + (s/s_{0}) \left\{ - \operatorname{sgn}(\lambda_{x} \lambda_{y}) \right\} \right\rangle \\ &= \frac{\operatorname{sgn} \, \Lambda}{2 \mathrm{i} \gamma s} \sum_{\lambda_{x}, \lambda_{y} \neq 0} \left[ \Theta \left( \left| \Lambda \right| + (s/s_{0}) \operatorname{sgn} \, \Lambda \right) \left| \lambda_{x}, \lambda_{y}, \Lambda + s/s_{0} \right\rangle \\ &- \Theta \left( \left| \Lambda \right| - (s/s_{0}) \operatorname{sgn} \, \Lambda \right) \left| \lambda_{x}, \lambda_{y}, \Lambda - s/s_{0} \right\rangle \right] \\ &= \iota_{0} \frac{\operatorname{sgn} \, \Lambda}{2 \mathrm{i} \gamma s} \left[ \Theta \left( \left| \Lambda \right| + (s/s_{0}) \operatorname{sgn} \, \Lambda \right) \left| \Lambda - s/s_{0} \right\rangle \right] \\ &= \iota_{0} \frac{\operatorname{sgn} \, \Lambda}{2 \mathrm{i} \gamma s} \left[ \Theta \left( \left| \Lambda \right| + (s/s_{0}) \operatorname{sgn} \, \Lambda \right) \left| \Lambda - s/s_{0} \right\rangle \right] \\ &= \iota_{0} \theta(s) |\Lambda \rangle. \end{split}$$

In going from line 3 to line 4, we have used the fact that the first and second terms are identical except that the signs in braces in the first term are all  $sgn(\lambda_x \lambda_y)$ , whereas all those in the second

term are  $-\operatorname{sgn}(\lambda_x \lambda_y)$ , so that in exactly one of the two terms these signs are all +1 and in the other they are -1.

**Theorem 2.**  $\iota$  as given in (65) satisfies

$${}^{\alpha'}\hat{\mathbb{S}}_i(s) \circ \iota = 0$$

for all choices of regularization parameter s and all choices of complexification parameter  $\alpha'$ , and independent of the choice of coefficients  $C(\Lambda; \Lambda')$ .

**Proof.** From equation (57), for all  $|\Lambda\rangle$ , we have

$$\begin{split} \overset{\alpha'}{\mathbb{S}}_{x}(s) \circ \iota |\Lambda\rangle &= \frac{\gamma}{2} |\hat{v}|^{1/2} \left( (\gamma \hat{\theta}_{x}(s) + \mathrm{i}\alpha') |\hat{v}| (\hat{\theta}_{y}(s) - \hat{\theta}_{z}(s)) \right. \\ &+ (\hat{\theta}_{y}(s) - \hat{\theta}_{z}(s)) |\hat{v}| (\gamma \hat{\theta}_{x}(s) + \mathrm{i}\alpha') \right) |\hat{v}|^{1/2} \cdot \cdot \left( \sum_{\Lambda' \in \mathbb{R}_{\kappa}} C(\Lambda'; \Lambda) \iota_{0} |\Lambda'\rangle \right) \\ &= \frac{\gamma}{2} \sum_{\Lambda' \in \mathbb{R}_{\kappa}} C(\Lambda'; \Lambda) |\hat{v}|^{1/2} \left( (\gamma \hat{\theta}_{x}(s) + \mathrm{i}\alpha') |\hat{v}| (\hat{\theta}_{y}(s) - \hat{\theta}_{z}(s)) \right. \\ &+ (\hat{\theta}_{y}(s) - \hat{\theta}_{z}(s)) |\hat{v}| (\gamma \hat{\theta}_{x}(s) + \mathrm{i}\alpha') \right) |\hat{v}|^{1/2} \circ \iota_{0} |\Lambda'\rangle \\ &= \frac{\gamma}{2} \sum_{\Lambda' \in \mathbb{R}_{\kappa}} C(\Lambda'; \Lambda) \iota_{0} \circ |\hat{v}|^{1/2} \left( (\gamma \hat{\theta}(s) + \mathrm{i}\alpha') |\hat{v}| (\hat{\theta}(s) - \hat{\theta}(s)) \right. \\ &+ (\hat{\theta}(s) - \hat{\theta}(s)) |\hat{v}| (\gamma \hat{\theta}(s) + \mathrm{i}\alpha') \right) |\hat{v}|^{1/2} |\Lambda'\rangle = 0 \end{split}$$

whence  ${}^{\alpha'}\hat{\mathbb{S}}_{z}(s) \circ \iota = 0$  for all s and  $\alpha'$ . Similarly,  ${}^{\alpha'}\hat{\mathbb{S}}_{y}(s) \circ \iota = {}^{\alpha'}\hat{\mathbb{S}}_{z}(s) \circ \iota = 0$  for all s and  $\alpha'$ .

Note that if *any other ordering* of  $\hat{\mathbb{S}}^i$  had been chosen in (57), this theorem would still hold. Furthermore, for the case  $\alpha' = -\alpha$ , this theorem implies that not only  $\hat{\mathbb{S}}_i \equiv {}^{\alpha} \hat{\mathbb{S}}_i(s_0)$  annihilates  $\iota$ , but also its adjoint  $\hat{\mathbb{S}}_i^{\dagger} \equiv {}^{-\alpha} \hat{\mathbb{S}}^i(s_0)$ . This contrasts with the full theory analysis in [15], where one only expects it to be possible for an embedding to be annihilated by one of  $\widehat{\mathbb{S}[f,g]}$ ,  $\widehat{\mathbb{S}[f,g]}$ , not both. Thus, the condition satisfied by  $\iota$  in the Bianchi I case is much stronger. The possibility of this was expected due to equation (46) in the classical theory, and this will be discussed in section 5.

Consistency with classical theory. It may seem puzzling that canonical residual automorphism covariance of  $\iota$  implies that its image satisfies our quantum isotropy condition: is not the former simply a condition of consistency with gauge symmetry, whereas the latter is an actual physical restriction on states? It may seem equally puzzling that it simultaneously implies that the adjoint of our isotropy condition is satisfied on the image of  $\iota$ .

These puzzles are resolved if one carefully translates these logical relations to the classical theory, where we will see that it holds as well. The canonical residual automorphism covariance of  $\iota$  implies that the image of  $\iota$  is invariant under the identity component of this group, the proper anisotropic dilatations. The classical analogue of imposing invariance under a unitary flow in quantum theory,  $e^{t\hat{X}}|\Psi\rangle = |\Psi\rangle$ , is to impose that the corresponding *generators* be zero:  $\hat{X}|\Psi\rangle = 0 \rightsquigarrow X \approx 0$ . The proper anisotropic dilatations are the flows on space generated by vector fields of the form  $\mathbf{X}_{t_x,t_y} := t_x x \frac{\partial}{\partial x} + t_y y \frac{\partial}{\partial y} - (t_x + t_y) z \frac{\partial}{\partial z}$ . The corresponding canonical

generators on the phase space are thus

$$X_{t_{x},t_{y}} = \frac{1}{\kappa\gamma} \int_{\mathcal{V}} A_{a}^{i} \mathcal{L}_{\mathbf{X}_{t_{x},t_{y}}} \tilde{E}_{i}^{a} d^{3}x = \frac{1}{\kappa\gamma} \left( -t_{x}(pc)_{x} - t_{y}(pc)_{y} - (-t_{x} - t_{y})(pc)_{z} \right)$$

$$= \frac{1}{\kappa\gamma} \left( (pc)_{z} - (pc)_{x} \right) t_{x} + \frac{1}{\kappa\gamma} \left( (pc)_{z} - (pc)_{y} \right) t_{y}$$

$$= \frac{-\mathbb{S}_{y}}{\kappa\gamma(pc)_{y}} t_{x} + \frac{\mathbb{S}_{x}}{\kappa\gamma(pc)_{x}} t_{y} = \frac{-\mathbb{S}_{y}}{\kappa\gamma\left((pc)_{y} + i\alpha\operatorname{vol}(\mathbf{p})\right)} t_{x} + \frac{\mathbb{S}_{x}}{\kappa\gamma\left((pc)_{x} + i\alpha\operatorname{vol}(\mathbf{p})\right)} t_{y}.$$

$$= \frac{-\overline{\mathbb{S}}_{y}}{\kappa\gamma\left((pc)_{y} - i\alpha\operatorname{vol}(\mathbf{p})\right)} t_{x} + \frac{\overline{\mathbb{S}}_{x}}{\kappa\gamma\left((pc)_{x} - i\alpha\operatorname{vol}(\mathbf{p})\right)} t_{y}. \tag{66}$$

The key point is that these generators are not constraints—anisotropic dilatations do not approach the identity at infinity, so that they are not generated by the diffeomorphism constraint. Thus, their vanishing imposes a non-trivial restriction on the physical degrees of freedom. In fact, it is immediate from the above form that the vanishing of the above generators for all  $t_x$ ,  $t_y$  is equivalent to  $\mathbb{S}_x \approx \mathbb{S}_y \approx 0$ , which is equivalent to  $\mathbb{S}_i \approx 0$  for all i—our classical isotropy condition. At the same time, it is equivalent to  $\overline{\mathbb{S}}_i \approx 0$ .

Imposition of intertwining of signed volume and Hubble operator. Imposition of canonical residual automorphism covariance and quantum isotropy has not yet uniquely determined the embedding  $\iota$ . But this was expected: these conditions have only restricted the *image* of  $\iota$ . As noted in [15], in order to achieve uniqueness of  $\iota$ , one expects to impose two more conditions, such as the intertwining of two operators. The basic variables in the isotropic theory are pand c, so it is natural to try to impose intertwining of corresponding operators with appropriate operators in the Bianchi I theory. One can indeed require that  $\iota$  intertwine  $\hat{p}$  with  $\hat{v}^{2/3}$  in Bianchi I, which is equivalent to requiring that  $\iota$  intertwine the signed volume  $\hat{v}$  in both theories. However, c has no operator analogue in the quantum theory, but rather only exponentials of c have operator analogues. Because of this, it is natural to instead require intertwining of an appropriate one-parameter family of exponentials of c, or operators constructed therefrom. We choose to require intertwining of the regularized isotropic Hubble rate  $\theta(s)$  (58) with one of the regularized directional Hubble rates (38)—specifically, we arbitrarily choose  $\theta_z(s)$  for this purpose. With this condition imposed, we shall see that  $\iota$  is uniquely determined up to an overall constant, and will then automatically intertwine  $\hat{\theta}(s)$  with the other directional Hubble rates as well. Indeed, we shall see that the resulting unique  $\iota$  will satisfy basically every property that could be desired from such an embedding.

Let  $Cyl_S$  denote the space of finite linear combinations of volume eigenstates in the isotropic theory, so that its algebraic dual,  $Cyl_S^*$ , may be identified with distributional states which include possibly non-normalizable linear combinations of volume eigenstates.

**Theorem 3.** There exists an embedding  $\iota$  from isotropic LQC states,  $\text{Cyl}_S^*$ , to Bianchi I quantum states,  $\text{Cyl}_{BI}^*$ , that (a) is covariant under all canonical residual automorphisms, (b) intertwines  $\hat{v}$  in the two theories, and (c) intertwines  $\hat{\theta}(s)$  with  $\hat{\theta}_z(s)$  for all s. This embedding is furthermore unique up to a (physically irrelevant) overall constant, and is given explicitly by  $\iota = C\iota_0$  for some  $C \in \mathbb{C}$ .

**Proof.** From equation (65), condition (a) imposes that  $\iota$  be of the form

$$\iota |\Lambda 
angle = \sum_{\Lambda' 
eq 0} C(\Lambda; \Lambda') \iota_0 |\Lambda' 
angle$$

for some  $C(\Lambda; \Lambda')$ . Condition (b) then forces  $C(\Lambda; \Lambda') = C(\Lambda)\delta_{\Lambda,\Lambda'}$  for some  $C(\Lambda)$ , and, finally, condition (c) forces  $C(\Lambda)$  to be a constant C.

The overall constant C is not a physical ambiguity, because quantum states have meaning only up to rescaling. Hence the embedding is physically unique, as was expected from the analysis of [15, 16]. From now on we set  $\iota$  to be equal to the embedding so selected, choosing C=1, so that

$$\iota|\Lambda\rangle = \iota_0|\Lambda\rangle = \sum_{\lambda_x, \lambda_y \neq 0} |\lambda_x, \lambda_y, \Lambda\rangle. \tag{67}$$

This is the Bianchi I analogue of what we have called the *volume embedding* in the full theory [15].

*Remark.* In selecting the unique embedding  $\iota$  above, we have required that it intertwine  $\hat{\theta}(s)$  with  $\hat{\theta}_z(s)$  for all s. One can alternatively require that, for all s, the more basic shift operators  $\hat{\Delta}(s)$  intertwine with a slight modification of  $\hat{\Delta}_z(s)$ , namely  $\hat{\Delta}'_i(s) := \exp\left(\frac{-ip_ic_is}{2v}\right)$ , also unitary, for, e.g. i = z. The resulting selected embedding is again the same. For this reason, these alternative shift operators are arguably more natural building blocks for the Bianchi I theory. Indeed, one could construct a Hamiltonian constraint operator from these alternative shift operators, and the result would be equivalent to the one used here and in [28] when acting on states  $|\lambda\rangle$  with sufficiently large volume. We have not used this alternative simply in order to be consistent with [28].

#### 4.4. Why the arguments against the volume embedding don't apply in the case of Bianchi I

In the full theory paper [15], we gave two arguments against the use of the volume embedding in the general case. Here, we address each of them, and show they do not apply in the simpler case of embedding into Bianchi I. First, we noted that the superposition which defines the volume embedding is in no way peaked on any geometries which are homogenious and isotropic. Since Bianchi I is homogeneous, we only have to address the apparent lack of isotropy in the target of the embedding (67). It is clear from (67) that, for each volume eigenstate  $|\Lambda\rangle$ ,  $\iota|\Lambda\rangle$  is a superposition of states  $|\lambda_x,\lambda_y,\Lambda\rangle$  for which the condition  $\lambda_x=\lambda_y=\lambda_z$  is *not* satisfied. However, this condition merely describes the dimensions of the fiducial cell; it has nothing to do with the isotropy of the phase space variables  $(q_{ab},K_{ab})$ . Rather, the correct isotropy condition is the one that been the subject of this paper: that states should be annihilated by the operators (57). From theorem 2 we know that  $\iota$  in fact does map all isotropic states into the isotropic sector of Bianchi I.

The second objection was that the definition of the volume embedding depends critically on the choice of basis used to define it. However, in the present Bianchi I context, there is no ambiguity at all in the embedding. As already shown above,  $\iota$  is (up to an overall constant) the unique embedding which is covariant under canonical residual automorphisms and which intertwines the signed volume and any one of the directional Hubble rates.

#### 4.5. Additional properties of the embedding

For each s,  $\iota$  intertwines all of the directional Hubble rates  $\hat{\theta}_i(s)$  with  $\hat{\theta}(s)$ . This follows from the fact that  $\iota = \iota_0$ , the volume embedding, and lemma 1.

 $\iota$  intertwines the Hamiltonian constraint operators of the isotropic and Bianchi I models. This is immediate from the expressions (40) and (59) for these Hamiltonian constraint operators, together with the properties  $\hat{v} \circ \iota = \iota \circ \hat{v}$  and  $\hat{\theta}_i(s) \circ \iota = \iota \circ \hat{\theta}(s)$  noted above.

*ι* is the adjoint of the projector of Ashtekar and Wilson-Ewing. In [28], Ashtekar and Wilson-Ewing define a projector from Bianchi I states to isotropic LQC states given by

$$\langle \Lambda | \hat{\mathbb{P}} \Psi \rangle = (\hat{\mathbb{P}} \Psi)(\Lambda) = \sum_{\lambda_x, \lambda_y} \Psi(\lambda_x, \lambda_y, \Lambda) = \sum_{\lambda_x, \lambda_y} \langle \lambda_x, \lambda_y, \Lambda | \Psi \rangle$$

for all  $\Psi$ , so that

$$\langle \Lambda | \hat{\mathbb{P}} = \sum_{\lambda_x, \lambda_y} \langle \lambda_x, \lambda_y, \Lambda |$$

and hence

$$\hat{\mathbb{P}}^\dagger |\Lambda
angle = \sum_{\lambda_x,\lambda_y} |\lambda_x,\lambda_y,\Lambda
angle = \iota |\Lambda
angle$$

whence  $\hat{\mathbb{P}}^{\dagger} = \iota$ .

Technical remark. Though  $\hat{\mathbb{P}}$  maps normalizable states in the Bianchi I Hilbert space  $\mathcal{H}$  to normalizable states in the isotropic Hilbert space  $\mathcal{H}_S$ , it is unbounded and hence only densely defined. As a consequence, its adjoint in the sense of a densely defined map  $\mathcal{H}_S \to \mathcal{H}$  need not, and in fact does not, exist. However, the adjoint in the algebraic dual sense always exists. The domain of  $\hat{\mathbb{P}}$  can be taken to be, for example,  $\text{Cyl}_{BI}$ ; with this choice, its range is  $\text{Cyl}_S$ . The adjoint in the algebraic dual sense,  $\hat{\mathbb{P}}^{\dagger}: \text{Cyl}_S^* \to \text{Cyl}_{BI}^*$  can then be restricted to a map  $\hat{\mathbb{P}}^{\dagger}: \mathcal{H}_S \to \text{Cyl}_{BI}^*$ . This is the map which equals our selected embedding  $\iota$  up to constant rescaling, mapping all non-zero states in  $\mathcal{H}_S$  into non-normalizable states in  $\text{Cyl}_{BI}^*$ .

#### 5. Origins of the embedding properties

In contrast to what is expected in the full theory [15], we have seen above that, for the embedding into Bianchi I, the following holds:

- (a) Not only is it possible to impose the quantization of the symmetry conditions (47) consistently in the quantum theory, but also possible to simultaneously impose their adjoint. Furthermore, a natural embedding of the quantum isotropic model into the common kernel of the quantum conditions and their adjoint exists.
- (b) Every operator of interest preserves the image of this natural embedding, and so is intertwined with some operator on  $\mathcal{H}_{\mathcal{S}}$  which turns out to be exactly the corresponding operator in the isotropic model.

These are surprisingly strong results. The first result implies that the quantization of the real and imaginary parts of  $\mathbb{S}_i$ — $\widehat{\operatorname{Re}}\, \mathbb{S}_i := \frac{1}{2}(\mathbb{S}_i + \mathbb{S}_i^{\dagger})$  and  $\widehat{\operatorname{Im}}\, \mathbb{S}_i := \frac{1}{2i}(\mathbb{S}_i - \mathbb{S}_i^{\dagger})$ —each annihilate the image of  $\iota$ . As first argued by Dirac [32], it is physically correct to impose a given system of real constraints strongly in quantum theory only if it forms a *first class system*. Do  $\operatorname{Re}\, \hat{\mathbb{S}}_i$  and  $\operatorname{Im}\, \hat{\mathbb{S}}_i$  form such a system? *Indeed they do*. This is equivalent to none other than the Poisson bracket (51).

In the following, we will see that the second result is likewise foreshadowed by classical Poisson brackets that indicate that, in fact, one expects the second result to be true for *every operator invariant under proper anisotropic dilatations*, and thus in particular for every operator invariant under residual automorphisms. Finally, we note that the Poisson brackets foreshadowing both of the above results hold thanks to the fact that  $\overline{\mathbb{S}}$  is proportional to  $\mathbb{S}$  with

coefficient smooth and non-vanishing everywhere, and trace the source of this to an observation about the physics of the Bianchi I phase space.

### 5.1. Poisson brackets indicating that $\iota$ should intertwine all proper-dilatation invariant operators

We here prove that any function F on the Bianchi I phase space invariant under proper anisotropic dilatations—and hence in particular any F invariant under residual automorphisms—satisfies

$$\{F, \mathbb{S}_i\} = \sum_j \lambda_i{}^j \mathbb{S}_j \tag{68}$$

for some matrix of phase space functions  $\lambda_i^j$ . This leads to the expectation that an appropriate quantization of each such quantity will preserve the quantum isotropic sector, hence preserve the image of the embedding, and therefore be intertwined with corresponding operators in the isotropic theory, a fact which we have already seen is true for F equal to the volume of the fiducial cell, the directional Hubble rates, and the Hamiltonian constraint operators<sup>9</sup>.

Let us begin with a general argument that the analogue of (68) in the full theory almost holds. This will allow us to see precisely the special property of the Bianchi I phase space that enables the argument to be completed. Suppose we are given a function F on the full theory phase space  $\Gamma_{\text{Full}}$  which is invariant under all spatial diffeomorphisms and local gauge rotations—that is, invariant under all automorphisms of the SU(2) principal fiber bundle. Let  $\overline{\Gamma_{\text{Full}}}$  be the bundle-automorphism-covariant homogeneous isotropic sector, defined as the set of points  $\eta \in \Gamma_{\text{Full}}$  such that  $\mathbb{S}[f,g](\eta) = 0$  for all f,g. From [15],  $\eta \in \Gamma_{\text{Full}}$  if and only if, for one of the three homogeneous-isotropic symmetry groups  $\mathcal{G}$  (Euclidean group, SO(4), or SO(3,1)), there exists some action  $\rho$  of  $\mathcal{G}$ , via bundle automorphisms, such that  $\rho(\alpha)\eta=\eta$  for all  $\alpha \in \mathcal{G}$ . Because F is automorphism invariant, its Hamiltonian flow cannot map one out of the symmetric sector  $\overline{\Gamma_{\text{Full}}}$ . Heuristically, one can see this because, in order for the flow of F to map a point in  $\overline{\Gamma_{\text{Full}}}$  out of itself, F would need to determine 'where' the inhomogeneity or 'in which direction' the anisotropy arises. But because F is invariant under diffeomorphisms and gauge rotations, this is not possible. More explicitly, let  $\eta \in \overline{\Gamma_{\text{Full}}}$  be given, let  $\mathcal{G}$  be the corresponding homogeneous-isotropic symmetry group, and let  $\rho$  be the corresponding action of  $\mathcal{G}$ . Let  $\Phi_F^t: \Gamma_{\text{Full}} \to \Gamma_{\text{Full}}$  denote the Hamiltonian flow generated by F on  $\Gamma_{\text{Full}}$ . Because both F and the Poisson brackets on  $\Gamma_{\text{Full}}$  are automorphism covariant, so is  $\Phi_F^t$  for each t, so that  $\varphi \circ \Phi_F^t = \Phi_F^t \circ \varphi$  for all automorphisms  $\varphi$  and all  $t \in \mathbb{R}$ . Thus, in particular, for all  $\alpha \in \mathcal{G}$  and all  $t \in \mathbb{R}$ , we have

$$\rho(\alpha)\Phi_F^t(\eta) = \Phi_F^t(\rho(\alpha)\eta) = \Phi_F^t(\eta)$$

so that  $\Phi_F^t(\eta) \in \overline{\Gamma_{\text{Full}}}$  as well. Thus  $\mathbb{S}[f,g](\Phi_F^t(\eta)) = 0$  for all t. Taking the derivative with respect to t and setting t to zero yields

$${F, \mathbb{S}[f,g]}(\eta) = 0$$

<sup>&</sup>lt;sup>9</sup> The full theory paper [15] also includes a notion of average spatial curvature which is invariant under gauge and diffeomorphisms. This is identically zero in the present Bianchi I framework and so is also (trivially) intertwined here.

for all f, g, and all  $\eta \in \overline{\Gamma_{\text{Full}}}$ . As  $\overline{\Gamma_{\text{Full}}}$  is the zero set of  $\mathbb{S}[f, g]$  for all f, g, and since the topology of  $\Gamma_{\text{Full}}$  is trivial, it follows that

$$\{F, \mathbb{S}[f, g]\} = \mathbb{S}[h, k] + \overline{\mathbb{S}[\tilde{h}, \tilde{k}]}$$

$$\tag{69}$$

for some  $h, k, \tilde{h}, \tilde{k}$  depending on f and g and possibly the phase space point.

The above argument goes through also for the Bianchi I case, with minimal modification. Let  $\Gamma$  denote the Bianchi I phase space as in section 2. The only modifications required to adapt the above argument to this case are the following:

- (a) The full group of bundle automorphisms is replaced by the canonical residual automorphisms. Aut $_R^C$ .
- (b) Instead of three possibilities for the symmetry group  $\mathcal{G}$ , there is only one, namely the residual rotation group,  $Rot_R$ —that part of the Euclidean group with well-defined and non-trivial action in the Bianchi I context.

That is, in the Bianchi I case one need only require that F, now a function on  $\Gamma$ , be invariant under  $\operatorname{Aut}_R^C$ . Additionally, for all  $\eta \in \Gamma$ , by theorem  $1, \mathbb{S}_i(\eta) = 0$  (i.e.  $\eta \in \overline{\Gamma}$ ) if and only if there exists some proper, and hence canonical, residual automorphism  $\varphi$  such that  $\eta$  is invariant under the action  $\rho(\pi) := \varphi \circ \pi \circ \varphi^{-1}$  of all  $\pi \in \operatorname{Rot}_R$ . This, combined with the invariance of F and the Poisson brackets under  $\operatorname{Aut}_R^C$ , allows the above argument in the full theory to be repeated unchanged in the Bianchi I case. Thus (69) holds also in the Bianchi I case, where it is more conveniently written as

$$\{F, \mathbb{S}_i\} = \sum_j \left( h_i{}^j \mathbb{S}_j + k_i{}^j \overline{\mathbb{S}}_j \right) \tag{70}$$

for some possibly phase space dependent  $h_i^j$ ,  $k_i^j$ . This is so far exactly analogous to the full theory. What is special in the Bianchi I case is equation (50), which allows (70) to be rewritten precisely in the form (68) claimed. Furthermore, equation (70) at any given phase space point  $\eta$  depends on F only in a neighborhood of  $\eta$ . As a consequence, the invariance of F under the full group of residual canonical automorphisms is not relevant for the validity of (70), but only invariance under the identity component of this group, namely the canonical anisotropic dilatations. That is, it is actually sufficient for F to be invariant under the smaller group of canonical anisotropic dilatations for (70) to hold. The volume of the fiducial cell, the directional Hubble rates, and the Hamiltonian constraint are all examples of such F's.

Explicit calculation in cases of interest. We here explicitly calculate the matrix of phase space functions  $\lambda^i_j$  in (68) for the cases of F corresponding to the operators already shown to be intertwined by the embedding  $\iota$ . We do this both for concreteness, as well as to perform a check on the general arguments above.

The volume of the fiducial cell. From the expressions (16), (44), (47), and  $\{c^i, p_j\} = \kappa \gamma \delta^i_j$ , one calculates

$$\{\mathbb{S}^{i}, \text{vol}(\mathbf{p})\} = \frac{\kappa \gamma}{2} \frac{1}{\gamma \theta_{i} + i\alpha} \mathbb{S}^{i}. \tag{71}$$

The directional Hubble rates. Similarly, from the definition (18),

$$\{\mathbb{S}^{i}, \theta_{k}\} = -\frac{\kappa}{2 \operatorname{vol}(\mathbf{p})} \frac{\gamma \theta_{k} + i\alpha}{\gamma \theta_{i} + i\alpha} \mathbb{S}^{i}. \tag{72}$$

The Hamiltonian constraint. From equation (20), using  $N = \text{vol}(\mathbf{p})^n$  from equation (40), and using the above two Poisson brackets, we have

$$\{\mathbb{S}^{i}, H_{g}\} = \frac{\operatorname{vol}(\mathbf{p})^{n}}{2(\gamma\theta_{i} + \mathrm{i}\alpha)} \left(\frac{1 - n}{\gamma} \sum_{j < k} \theta_{j} \theta_{k} + 2\mathrm{i}\alpha \sum_{j=1}^{3} \theta_{j}\right) \mathbb{S}^{i}$$

$$= \frac{1}{\gamma\theta_{i} + \mathrm{i}\alpha} \left(\frac{\gamma(n-1)}{2\operatorname{vol}(\mathbf{p})} H_{g} + \mathrm{i}\alpha \operatorname{vol}(\mathbf{p})^{n} \sum_{j=1}^{3} \theta_{j}\right) \mathbb{S}^{i}. \tag{73}$$

#### 5.2. Deeper source of surprising simplifications in the Bianchi I case

At the start of this section, we have summarized a number of surprisingly congruous features of the quantum isotropic symmetric sector of Bianchi I and a natural embedding of the quantum isotropic theory into it. In section 5.1 we have exhibited reason to expect that these features extend even further. Furthermore, the argument above in section 5.1, as well as the arguments in section 3.1, show that all of these unexpected results, in the end, can be traced to the fact (50), that  $\overline{\mathbb{S}}_i$  and  $\mathbb{S}_i$  are proportional to each other with coefficient everywhere smooth and non-vanishing. Why does this property hold specifically in Bianchi I? This property is directly implied by the fact that the real part of the symmetry condition is proportional to the imaginary part by an everywhere smooth and real coefficient:

$$\operatorname{Re} \mathbb{S}_{i} = \left(\frac{\gamma \theta_{i}}{\alpha}\right) \operatorname{Im} \mathbb{S}_{i}. \tag{74}$$

This coefficient is non-vanishing throughout  $\Gamma$  except where  $c_i = 0$ . This proportionality is a reflection of the fact that the real and imaginary parts of the symmetry conditions  $\mathbb{S}_i \approx 0$  are not independent, but rather the imaginary part implies the real part, and almost vice versa.

Why are only half of the symmetry conditions independent? To see the answer to this question, we note that the fact that the spin-connection is flat means that the spatial geometry is unique up to diffeomorphism in Bianchi I—i.e. the triad  $\tilde{E}^a_i$  by itself has no diffeomorphism and gauge invariant information. This can also be seen more directly. Consider the action (10), (11) of the residual diffeomorphisms in the Bianchi I case. It is easy to see that this action acts transitively on the space of all non-degenerate densitized triads  $\tilde{E}^a_i = p_i \delta^a_i$  in Bianchi I. The same is also true for the space of all connections  $A^i_a = c^i \delta^i_a$  if one restricts to connections with no vanishing components. Thus,  $\tilde{E}^a_i$  by itself and  $A^i_a$  by itself (basically) each contain no diffeomorphism invariant information. Only the relation between them contains diffeomorphism invariant information. Because the symmetry condition  $S_i \approx 0$  is diffeomorphism invariant, this means that it implies no condition on  $\tilde{E}^a_i$  or  $A^i_a$  separately, but only a condition on their relation to each other. Thus, if the residual diffeomorphism freedom is used to completely fix  $\tilde{E}^a_i$  arbitrarily, the symmetry condition yields a condition on  $A^i_a$  only, or vice-versa, so that effectively the symmetry constraint is a constraint on only 'half' of the variables.

This last observation also resolves a tension in the fact that, as mentioned above, the set of constraint functions  $\{\text{Re }\mathbb{S}_i, \text{Im }\mathbb{S}_i\}$  are first class. This set imposes the diffeomorphism invariant part of the symmetry condition on both  $\tilde{E}_i^a$  and  $A_a^i$ , conjugate variables. Real-valued constraint functions imposing symmetry on conjugate variables normally would form a *sec-ond* class set, not a first class set [14–16]. However, as noted in the last paragraph, because

our symmetry conditions impose only the diffeomorphism invariant part of homogeneity and isotropy, in the present Bianchi I case, the conditions impose no conditions on either  $\tilde{E}^a_i$  or  $A^i_a$  separately, but only on the relation between the two. Thus, specifically in this Bianchi I case, no symmetry condition is imposed separately and simultaneously on any conjugate components of variables, so that the usual argument leading to the conclusion that the real and imaginary parts of the constraint functions should be second class does not apply.

#### 6. Discussion

In the work [15, 16], we introduced a gauge- and diffeomorphism-invariant—that is, principal-bundle-automorphism invariant—notion of homogeneous and isotropic states in full LQG, together with a strategy for constructing an embedding of LQC states into the space of such full theory states. We proposed that the resulting embedding be used to relate proposals for dynamics in full LQG with choices of dynamics in LQC, where observational consequences can be more easily calculated.

In the present paper, as a test, we have applied these ideas to the simpler case of embedding into Bianchi I, with surprising success. In this simpler context, the automorphism-invariant conditions for homogeneity and isotropy reduce to residual-automorphism-invariant conditions  $\mathbb{S}^i \approx 0$  for isotropy. They can be easily quantized in the manner analogous to that suggested for the full theory in [15, 16] and using the methods of [28], yielding operators  $\hat{\mathbb{S}}^i$ . These operators are non-Hermitian, and may be thought of as the 'holomorphic part' of the symmetry conditions in the Gupta–Bleuler sense.

Furthermore, we have shown that there exists a *unique* embedding, of isotropic LQC into Bianchi I states, satisfying the following three conditions:

- (a) It be covariant under all residual automorphisms with well-defined actions on quantum states—the canonical residual automorphisms.
- (b) It intertwine the signed volume operator in the two models.
- (c) It intertwine the regularized directional Hubble rate  $\hat{\theta}_z(s)$  in the Bianchi I model with the Hubble rate  $\hat{\theta}(s)$  in the isotropic model for all s.

The embedding  $\iota$  so selected then automatically satisfies the following further properties:

- It is annihilated by the quantum isotropy conditions  $\hat{\mathbb{S}}_i$ —that is, it is an embedding into the sector of quantum isotropy.
- It intertwines *all* of the directional Hubble rates  $\hat{\theta}_i$  with  $\hat{\theta}$ .
- It intertwines the Hamiltonian constraint operators in the isotropic and Bianchi I models.
- It is the adjoint of the projector from Bianchi I states to isotropic states introduced by Ashtekar and Wilson-Ewing in [28].

In particular,  $\iota$  intertwines every operator of interest in the isotropic and Bianchi I models. From classical analysis, we in fact have seen that we expect *all* canonical residual automorphism invariant operators in the Bianchi I and isotropic models, if appropriately quantized, to be intertwined by  $\iota$ . Equally surprisingly, and perhaps at the root of this, we have seen that  $\iota$  is not only annihilated by  $\hat{\mathbb{S}}_i$ , *but also by the adjoints*  $\hat{\mathbb{S}}_i^{\dagger}$ —by *both* the 'holomorphic' and 'anti-holomorphic' parts of the symmetry conditions. In section 5, we traced these last two surprising results to the fact that, in Bianchi I, Re  $\mathbb{S}_i$  is proportional to Im  $\mathbb{S}_i$  with coefficient everywhere finite and smooth, a fact which does not hold in the full theory [15]. Though, in the full theory, we thus expect the obvious interesting operators to not preserve the quantum homogeneous isotropic sector, nevertheless, in this same work [15] we have laid out a strategy to handle the expected resulting added complication in this case.

It would be interesting to investigate covariance of  $\iota$  also with respect to more general diffeomorphisms. It may well be possible to define a natural action of diffeomorphisms more general than the residual ones in Bianchi I that preserve the gauge-fixing. Although the Bianchi I model is usually introduced by gauge fixing, this is not necessary. One can instead (1) impose Bianchi I symmetry up to diffeomorphism in the full gravitational phase space, (2) pull-back the symplectic structure to this subspace, and then (3) divide by the kernel of the resulting symplectic structure. This kernel will consist in diffeomorphism directions in the phase space, so that each point in the final phase space is a diffeomorphism-equivalence class of full gravitational data. The result will be isomorphic to the usual Bianchi I phase space, but with no gauge-fixing. Indeed, in the present paper, the isotropic model was derived from the Bianchi I model in precisely this way, allowing a natural action of anisotropic dilatations on the resulting phase space. These break the usual gauge fixing in the isotropic case, and so normally would not be defined. It would be interesting to see which additional spatial diffeomorphisms might acquire a natural action in the quantum theory by pursuing an analogous strategy in Bianchi I. We leave this as an open question. However, since the action of any such further diffeomorphism would be made possible by allowing action within equivalence classes, which correspond to single points in the phase space, it seems likely that it would coincide with the action of one of the canonical residual diffeomorphisms already defined in this paper. If so, then  $\iota$  would be covariant also with respect to any such additional diffeomorphisms.

A further question is covariance with respect to *space–time* diffeomorphisms. Space–time diffeomorphisms in the direction normal to the Cauchy slice are generated by the Hamiltonian constraint smeared with different lapses. From equation (20), we see that Hamiltonian constraints smeared with *arbitrary*, phase space-independent lapse, when restricted to the Bianchi I phase space, are all proportional to each other, so that the operator corresponding to any such Hamiltonian constraint equals a constant times the operator (40) for n = 0. This operator has already been shown to be intertwined by our  $\iota$ . Thus  $\iota$  is arguably covariant also with respect to arbitrary space–time diffeomorphisms normal to the Cauchy surface.

Summarizing, it may be possible to show that  $\iota$  is covariant under a much larger class of space-time diffeomorphisms than explicitly claimed above. Of course, in order to make a larger claim than we have done, it would be important to check that the action of the diffeomorphisms is consistent with the hypersurface deformation algebra (Dirac algebra) [33–35]. For the diffeomorphisms considered above, we expect this to be the case. For example, the hypersurface deformation algebra states the commutator of two Hamiltonian constraints with phase space-independent lapse should be proportional to a diffeomorphism constraint. In Bianchi I, the diffeomorphism constraint is identically zero, so this becomes the condition that all such Hamiltonian constraints commute. The fact, noted in the prior paragraph, that the operators corresponding to all such Hamiltonian constraints are proportional to each other means that this particular part of the hypersurface deformation algebra is indeed satisfied. One might expect the other parts of the algebra (appropriately formulated in terms of finite diffeomorphisms) to be satisfied simply because of the natural way that the action of spatial diffeomorphisms is constructed in the quantum theory. One could argue that the correctness of the commutator between two Hamiltonian constraints here summarized is too trivial of a check, because it is zero. This might be remedied by considering also phase-space dependent lapses, such as those corresponding to  $n \neq 0$  in equation (40), which lead to Hamiltonian constraints with generally non-vanishing Poisson brackets. Investigations along these lines might provide an interesting new avenue to pursue the issues related to space—time covariance raised in [33, 36, 37].

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#### Data availability statement

No new data were created or analysed in this study.

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