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Loop quantum cosmology: I. Kinematics

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Abstract. The framework of quantum symmetry reduction is applied to loop quantum gravity with respect to transitively acting symmetry groups. This allows us to test loop quantum gravity in a large class of minisuperspaces and to investigate its features—e.g. the discrete volume spectrum—in certain cosmological regimes. Contrary to previous studies of quantum cosmology (minisuperspace quantizations) the symmetry reduction is carried out not at the classical level but on an auxiliary Hilbert space of the quantum theory before solving the constraints. Therefore, kinematical properties like volume quantization survive the symmetry reduction. In this first part of a series of papers the kinematical framework, i.e. implementation of the quantum symmetry reduction and quantization of Gauß and diffeomorphism constraints, is presented for Bianchi class A models as well as locally rotationally symmetric and spatially isotropic closed and flat models.

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1. Introduction

One of the main applications of general relativity has always been the study of cosmological models, i.e. of solutions which allow a transitive group of space isometries. This symmetry condition reduces the infinite number of degrees of freedom of general relativity to finitely many ones for these homogeneous minisuperspace models [1, 2], leading to their extensive use as test models for a quantum theory of gravity. In this respect they are similar to quantum mechanical models with the role of the Schrödinger equation played by the Wheeler–DeWitt equation [1], which is the quantized Hamiltonian constraint of general relativity. This equation is a hyperbolic differential equation involving the scale factor of the universe, which plays a role analogous to a time variable. It remains hyperbolic after small perturbations of the homogeneous metrics [3].

Given the lack of a complete quantum theory of gravity, this approach of quantization *after* symmetry reduction has long been the only possibility for studying quantum effects in cosmology, which are believed to have a large impact on the development of a universe, at least in its very early stages. But now there are candidates for such a quantum theory with powerful techniques, and it is legitimate to ask what these theories have to say about such questions. The most ambitious approach which is claimed to provide a quantum theory of gravity is string theory [4]. In the cosmological context it has been applied to the study of inflationary models because its field content is different from general relativity [5–7]. A second novelty is a scale factor duality [8] which relates universes of small and large scale. But the approach to quantum cosmology is the same as that of general relativity, only the Einstein–Hilbert action is

changed by some effective terms. Thus, concerning quantization of the metric, as yet nothing conceptually new has come into play through using the ideas of string theory.

In a second approach to quantum gravity, loop quantum gravity [9], the situation is different. Basic geometric quantities have been quantized [10–14] and found to have discrete spectra. Their eigenstates are spin network states, a discrete structure of space. Continuous space is regarded as an approximate concept at large scales, which can be described by weave states [15]. Some preliminary considerations in the cosmological context using these weaves have appeared in [16]. Evidently, in such a situation, concepts like the hyperbolic differential equation with respect to the scale factor cannot remain true. The departure from those ideas of differential Wheeler–DeWitt equations can best be seen by looking at the quantization of the Wheeler–DeWitt operator in loop quantum gravity [17–19]. Unfortunately, this operator of the full theory remains poorly understood.

In the present paper we make use of symmetric, distributional states of loop quantum gravity which have been defined and investigated in [20]. Contrary to weaves, they are exactly symmetric, not only approximately at large scales. This fact guarantees that the number of degrees of freedom is reduced to finitely many ones as in classical symmetry reductions. Nevertheless, we impose the symmetry conditions in quantum theory, namely in the auxiliary Hilbert space of loop quantum gravity, and we can use all the techniques of loop quantum gravity for the investigation of cosmological models. In particular, spectra of geometric operators remain discrete. In these reduced models we then have to quantize and solve the reduced constraints, which will be done in the present paper for the kinematical ones. Concerning the more complicated Hamiltonian constraint, which leads to the Wheeler–DeWitt equation, our reduced models can provide helpful tests for its quantization [21] as well as solution.

In this paper the emphasis lies on the implementation of the kinematical framework. Besides providing the stage for future work this will serve us as a means to test some ideas of the symmetry reduction of [20]. In particular, the Higgs constraint ([20] and section 2) can be analysed more easily because there is just one Higgs vertex in the reduced model. Cosmological considerations will not appear in this paper, and therefore we will not bother ourselves with matter couplings.

The next section recalls the necessary material of [20] specialized to transitive group actions. Section 3 introduces some cosmological models classically as well as in their quantum symmetry reduced form. In section 4 we quantize and solve the Gauß constraints and in section 5 we do the same for the diffeomorphism constraints for these models.

2. Quantum symmetry reduction for transitive symmetry groups

In this section we provide the mathematical prerequisites for a quantum treatment of cosmological models. These are the classification of symmetric principal fibre bundles and invariant connections thereon [22] and the general framework of quantum symmetry reduction [20], both specialized to transitive actions of a symmetry group. This section thereby serves to fix our notation.

2.1. Invariant connections

Let $P(\Sigma, G, \pi)$ be a principal fibre bundle over the compact manifold Σ , which is regarded as a space manifold for canonical quantization, and with structure group G, which will be G = SU(2) for gravity formulated in real Ashtekar variables. On P there is a given transitivelyacting symmetry group S < Aut P of bundle automorphisms. To allow for group actions with rotational symmetry in addition to homogeneity, S can have a non-trivial isotropy (this

mathematical notion of isotropy should not be confused with the physical concept) subgroup F < S (fixing a point x_0 in Σ), which is up to conjugacy the same for all points in Σ due to transitivity of the action of S. Σ can be represented as $\Sigma \cong S/F$, and $\Sigma/S =: B = \{x_0\}$ is represented by a single point which can be chosen arbitrarily in Σ . The general framework demands that the coset space S/F is reductive [22], i.e. the Lie algebra of S can be decomposed as $\mathcal{L}S = \mathcal{L}F \oplus \mathcal{L}F_{\perp}$ with $\mathrm{Ad}_F \mathcal{L}F_{\perp} \subset \mathcal{L}F_{\perp}$. Important examples are semisimple groups S, in which case $\mathcal{L}F_{\perp}$ is the orthogonal complement of $\mathcal{L}F$ with respect to the Cartan–Killing metric, freely acting groups with $F = \{1\}$ and $\mathcal{L}F_{\perp} = \mathcal{L}S$, and semidirect products $S = N \rtimes F$ with $\mathcal{L}F_{\perp} = \mathcal{L}N$. We will encounter the last case when studying homogeneous models with a rotational isotropy subgroup F. N will then be a translational subgroup (isomorphic to one of the Bianchi groups) of S, and act freely and transitively.

The isotropy subgroup plays an important role in the classification of symmetric bundles and invariant connections [22]. It provides in the first place a map $F: \pi^{-1}(x_0) \to \pi^{-1}(x_0)$, by means of which group homomorphisms $\lambda_p: F \to G$ can be defined, for each point p in the fibre over x_0 , by means of $f(p) =: p \cdot \lambda_p(f)$ for all $f \in F$. By choosing a different point $p \cdot g$ in the fibre over x_0 such a homomorphism gets conjugated: $\lambda_{p \cdot g} = \operatorname{Ad}_{g^{-1}} \circ \lambda_p$. Therefore, for the following classifications only the conjugacy class $[\lambda]$ of a given homomorphism matters. But for homomorphisms from different conjugacy classes the S-actions on a given principal fibre bundle P are inequivalent, and therefore all S-symmetric principal fibre bundles are classified by a conjugacy class $[\lambda]$ of group homomorphisms $\lambda: F \to G$.

The next question is, given an S-symmetric principal fibre bundle P classified by $[\lambda]$, what is the general form of a $[\lambda]$ -invariant, i.e. invariant with respect to this classified action of S on P, connection on P? By using the Maurer–Cartan form θ_{MC} on S and an embedding $\iota: S/F \hookrightarrow S$ all such connections can be written in the form

$$\omega_{S/F} = \phi \circ \iota^* \theta_{MC} \tag{1}$$

where $\phi: \mathcal{L}F_{\perp} \to \mathcal{L}G$ is a linear map obeying the equation

$$\phi(\operatorname{Ad}_f(X)) = \operatorname{Ad}_{\lambda(f)}\phi(X) \tag{2}$$

for all $f \in F$, $X \in \mathcal{L}F_{\perp}$, and where $\lambda \in [\lambda]$ is chosen from the conjugacy class. In what follows, the map ϕ will be denoted as a Higgs field. The structure group G acts on ϕ by conjugation, which stems from the usual gauge transformation of a connection; the solution space of equation (2) is, however, invariant only with respect to the reduced structure group $Z_{\lambda} := Z_G(\lambda(F))$, the centralizer of $\lambda(F)$ in G. This fact leads to a partial gauge fixing which is manifest in all classical symmetry reductions: the reconstructed connection form $\omega_{S/F}$ is a Z_{λ} -connection and will in general depend explicitly on λ . As noted above, only the conjugacy class $[\lambda]$ plays a gauge-invariant role, and indeed after choosing a different $\lambda' \in [\lambda]$ we would reconstruct a gauge-equivalent connection. In classical symmetry reductions a fixed $\lambda \in [\lambda]$ is chosen once and for all leading to a breaking of the structure group from G to Z_{λ} .

2.2. Symmetric states

The basic idea of [20] is to use the reconstruction of invariant connections from the Higgs field to pull back a spin network function, which is a function on the space $\overline{\mathcal{A}}_{\Sigma}$ of generalized connections on Σ modulo gauge transformations, to a function on the space $\overline{\mathcal{A}}_{B} \times \overline{\mathcal{U}}_{B}$ of generalized connections and Higgs fields on the reduced manifold B. It was also shown there, how the functions on $\overline{\mathcal{A}}_{B} \times \overline{\mathcal{U}}_{B}$ can be interpreted as distributional states of the unreduced theory which are $[\lambda]$ -symmetric in the sense that their supports contain only $[\lambda]$ -invariant connections on Σ . Furthermore, it was shown that all symmetric states can be obtained in such a way.

In the case of transitively acting symmetry groups, $B = \{x_0\}$ consists of a single point and the space $\overline{\mathcal{U}}_B$ is finite-dimensional, whereas $\overline{\mathcal{A}}_B$ certainly makes no contribution. The reduced theory will hence only have finitely many degrees of freedom after a quantum symmetry reduction (analogously to the classical reduction).

There are some subtleties, because of the partial gauge fixing, which will show up in the solution space of equation (2). To start with, for each basis element of $\mathcal{L}F_{\perp}$ we will use a separate Higgs field component which will be described by using point holonomies [23] in the quantum theory. By using point holonomies with respect to the structure group G instead of Z_{λ} the partial gauge fixing can be undone. This is even mandatory, because point holonomies necessarily transform under the adjoint representation of the structure group, whereas Higgs fields will not necessarily transform under the adjoint representation of Z_{λ} . The space of point holonomies will, however, be the quantum configuration space only for freely acting symmetry groups. If F is non-trivial, the condition (2) will further constrain this space. More details will be given in the next section, and concerning solutions of equation (2) in the next part of this series [24].

3. Bianchi class A models, locally rotationally symmetric and isotropic models

Here we introduce the models we are interested in: Bianchi class A models constitute all homogeneous models with a freely acting symmetry group $(F = \{1\})$ which can be treated in a Hamiltonian formulation (Bianchi class B models violate the principle of symmetric criticality [25,26]). Some of them can be reduced further on by demanding rotational symmetry with one axis (F = U(1)) or even isotropy (F = SU(2)); in general this isotropy subgroup does not project to an SO(3)-action on P, although it does on Σ).

3.1. Bianchi class A models

Bianchi models describe all possible types of metrics which are homogeneous in space [27]. They have been discussed in a minisuperspace quantization, e.g. in [28]. The classical reduction in terms of complex Ashtekar variables has been carried out in [29]. Here we present the reduction for real Ashtekar variables in the framework described in the preceding section.

In the context of Bianchi models the transitive symmetry group acts freely on Σ , which implies that Σ can be identified with the group manifold S (up to a suitable compactification if S is non-compact). The three generators of $\mathcal{L}S$ are denoted as T_I , $1 \leq I \leq 3$, with the relations $[T_I, T_J] = c_{IJ}^K T_K$. Here c_{IJ}^K are the structure constants of $\mathcal{L}S$ fulfilling $c_{IJ}^J = 0$ for class A models by definition. The Maurer–Cartan form on S is given by $\theta_{MC} = \omega^I T_I$ with left invariant 1-forms ω^I on S which fulfill the Maurer–Cartan equations

$$d\omega^I = -\frac{1}{2}c^I_{JK}\omega^J \wedge \omega^K \,. \tag{3}$$

Due to $F=\{1\}$ all homomorphisms $\lambda\colon F\to G$ are given by $1\mapsto 1$, and we can use the embedding $\iota=\operatorname{id}\colon S/F\hookrightarrow S$. An invariant connection then takes the form $A=\phi\circ\theta_{\mathrm{MC}}=\phi_I^i\tau_i\omega^I=A_a^i\tau_i\mathrm{d}x^a$ with the matrices $\tau_j=-\frac{\mathrm{i}}{2}\sigma_j$ generating $\mathcal{L}SU(2)$ (σ_j are the Pauli matrices). The Higgs field is given by $\phi\colon\mathcal{L}S\to\mathcal{L}G$, $T_I\mapsto\phi(T_I)=:\phi_I^i\tau_i$ already in its final form, because the Higgs condition (2) is empty. By using the left invariant vector fields X_I obeying $\omega^I(X_J)=\delta^I_J$ and with Lie brackets $[X_I,X_J]=c^K_{IJ}X_K$ the momenta canonically conjugate to $A_a^i=\phi_I^i\omega_a^I$ can be written as $E_i^a=\sqrt{g_0}\,p_I^iX_I^a$ with p_I^I being canonically conjugate to ϕ_I^i . Here $g_0=\det(\omega_a^I)^2$ is the determinant of the left invariant metric $(g_0)_{ab}:=\sum_I\omega_a^I\omega_b^I$ on Σ which is used to provide the density weight of E_i^a . The symplectic

structure can be derived from

$$(\kappa \iota)^{-1} \int_{\Sigma} d^3 x \, \dot{A}_a^i E_i^a = (\kappa \iota)^{-1} \int_{\Sigma} d^3 x \, \sqrt{g_0} \, \dot{\phi}_I^i p_i^J \omega^I(X_J)$$
$$= (\kappa \iota)^{-1} V_0 \dot{\phi}_I^i p_i^J,$$

to obtain

$$\{\phi_I^i, p_I^J\} = \kappa \iota' \delta_I^i \delta_I^J \tag{4}$$

with the gravitational constant κ and the modified Immirzi parameter $\iota' := \iota V_0^{-1}$ in which we absorbed the volume $V_0 := \int_{\Sigma} d^3x \sqrt{g_0}$ of Σ measured in the invariant metric g_0 .

We proceed now by inserting the invariant connections and canonical dreibeine into the Gauß, vector and Hamiltonian constraints. But before doing so we show that the divergence of the density-weighted vector fields $\sqrt{g_0}X_I$, which appear in the Gauß constraint, vanishes. To that end we use a metric-independent duality transformation which assigns to an n-form $\omega = (n!)^{-1}\omega_{a_1...a_n} dx^{a_1} \wedge \cdots \wedge dx^{a_n}$ in D dimensions the components

$$(*\omega)^{a_{n+1}...a_D} := (n!)^{-1} \epsilon^{a_1...a_n a_{n+1}...a_D} \omega_{a_1...a_n}$$

of a density-weighted antisymmetric tensor, and, vice versa, to a density-weighted antisymmetric tensor X, the differential form

$$*X := [(D-n)!]^{-1} \epsilon_{a_1...a_n a_{n+1}...a_D} X^{a_1...a_n} dx^{a_{n+1}} \wedge \cdots \wedge dx^{a_D}.$$

Here, $\epsilon^{a_1...a_D}$ and $\epsilon_{a_1...a_D}$ are the metric independent ϵ -tensors in D dimensions with density weight 1 and -1, respectively. The divergence of $\sqrt{g_0}X_I$ can now be written as div $\sqrt{g_0}X_I = *d*(\sqrt{g_0}X_I) = *dB_I$ with

$$B_{I} := *(\sqrt{g_{0}}X_{I}) = \frac{1}{2}\epsilon_{abc}\sqrt{g_{0}}X_{I}^{a}dx^{b} \wedge dx^{c}$$

$$= \frac{1}{2}\epsilon_{JKL}\omega_{a}^{J}\omega_{b}^{K}\omega_{c}^{L}X_{I}^{a}dx^{b} \wedge dx^{c}$$

$$= \frac{1}{2}\epsilon_{IKL}\omega_{b}^{K}\omega_{c}^{L}dx^{b} \wedge dx^{c}$$

$$= \frac{1}{2}\epsilon_{IKL}\omega_{b}^{K}\wedge \omega_{c}^{L}dx^{b}$$

$$= \frac{1}{2}\epsilon_{IKL}\omega_{b}^{K}\wedge \omega_{c}^{L}dx^{c}$$

The exterior derivative of B_I can be calculated by using the Maurer–Cartan equations (3):

$$dB_{I} = -\epsilon_{IKL}\omega^{K} \wedge d\omega^{L} = \frac{1}{2}\epsilon_{IKL}c_{MN}^{L}\omega^{K} \wedge \omega^{M} \wedge \omega^{N}$$

$$= \frac{1}{2}c_{MN}^{L}\epsilon_{IKL}\epsilon^{KMN}\sqrt{g_{0}} d^{3}x$$

$$= \frac{1}{2}c_{MN}^{L}(\delta_{L}^{M}\delta_{I}^{N} - \delta_{I}^{M}\delta_{L}^{N})\sqrt{g_{0}} d^{3}x$$

$$= -c_{IL}^{L}\sqrt{g_{0}} d^{3}x.$$

In the last two calculations we used the identity

$$\sqrt{g_0} = \frac{1}{6} \epsilon_{IJK} \epsilon^{abc} \omega_a^I \omega_b^J \omega_c^K$$

for the determinant of the invariant metric in terms of left invariant 1-forms. The divergence of $\sqrt{g_0}X_I$ can now be read off as div $\sqrt{g_0}X_I = *dB_I = -c_{IL}^L\sqrt{g_0}$, i.e. it vanishes precisely for Bianchi class A models.

The Gauß constraint can now be calculated easily:

$$\mathcal{G}_{i} = (\kappa \iota)^{-1} \int_{\Sigma} d^{3}x (\partial_{a} E_{i}^{a} + \epsilon_{ijk} A_{a}^{j} E_{k}^{a})
= (\kappa \iota)^{-1} \int_{\Sigma} d^{3}x (p_{i}^{I} \operatorname{div} \sqrt{g_{0}} X_{I} + \sqrt{g_{0}} \epsilon_{ijk} \phi_{I}^{j} p_{k}^{I})
= (\kappa \iota')^{-1} (\epsilon_{ijk} \phi_{I}^{j} p_{k}^{I} - c_{IJ}^{J}).$$
(5)

For the next two constraints we will need the curvature of $A = \phi_I^i \tau_i \omega^I$. It is given by

$$F = dA + \frac{1}{2}[A, A]$$

$$= \phi_I^i \tau_i d\omega^I + \frac{1}{2} \epsilon_{ijk} \phi_I^i \phi_J^j \tau^k \omega^I \wedge \omega^J$$

$$= \frac{1}{2} (-\phi_I^i c_{JK}^I + \epsilon_{ijk} \phi_J^j \phi_K^k) \tau_i \omega^J \wedge \omega^K$$

again using the Maurer-Cartan equations. The components of the curvature are

$$F_{IJ}^i = -\phi_K^i c_{IJ}^K + \epsilon_{ijk} \phi_I^j \phi_J^k.$$

They are now used to calculate the vector constraint with a shift vector $N^a = N^I X_I^a$, N^I constant (the fact that the N^I are constant on Σ is a manifestation of a partial gauge fixing of diffeomorphisms by demanding them to respect the symmetry; this corresponds to choosing a special system of coordinates adapted to the symmetry):

$$\mathcal{V}_{a}N^{a} = (\kappa \iota)^{-1} \int_{\Sigma} d^{3}x \, F_{IJ}^{i} E_{i}^{J} N^{I}$$

$$= (\kappa \iota)^{-1} \int_{\Sigma} d^{3}x \sqrt{g_{0}} (-c_{IJ}^{K} \phi_{K}^{i} p_{i}^{J} + \epsilon_{ijk} \phi_{I}^{j} \phi_{J}^{k} p_{i}^{J}) N^{I}$$

$$= (\kappa \iota')^{-1} (-c_{IJ}^{K} \phi_{K}^{i} p_{i}^{J} + \phi_{I}^{j} \mathcal{G}_{i}) N^{I}$$

$$(6)$$

where the first term

$$\mathcal{D}_a N^a = -(\kappa \iota')^{-1} c_{II}^K \phi_K^i p_i^J N^I \tag{7}$$

is the diffeomorphism constraint. We note here that \mathcal{G} and \mathcal{D} are very similar: \mathcal{G} generates as gauge transformations conjugation in the internal SU(2) space, whereas \mathcal{D} generates conjugation in the homogeneous space S. Therefore, the constants appearing in the constraints are the structure constants ϵ_{ijk} of SU(2) and c_{JK}^I of S, respectively. We will say more about this point when we quantize and solve the diffeomorphism constraint in section S.

Finally, we calculate the Euclidean part of the Hamiltonian constraint. In real Ashtekar variables there is an additional term in the Lorentzian constraint [30], which can, however, be dealt with by the same methods as in [18] for the full theory. Therefore, we will not require its reduction explicitly. The Euclidean part (with density weight 2) is given by

$$\mathcal{H}^{(E)} = \epsilon_{ijk} F_{IJ}^i E_j^I E_k^J$$

$$= g_0(-\epsilon_{ijk} c_{IJ}^K \phi_K^i p_j^I p_k^J + \epsilon_{ijk} \epsilon_{ilm} \phi_I^l \phi_J^m p_j^I p_k^J)$$

$$= g_0(-\epsilon_{ijk} c_{IJ}^K \phi_K^i p_j^I p_k^J + \phi_I^j \phi_I^k p_i^J p_k^J - \phi_I^k \phi_I^j p_i^J p_k^J). \tag{8}$$

3.2. Locally rotationally symmetric and isotropic models

On some of the Bianchi models additional symmetry conditions can be imposed. If there is an isotropy subgroup $F \cong U(1)$ of the symmetry group S, one obtains locally rotationally symmetric models (LRS models, [27,31]; we use the term LRS only for the restricted class of F = U(1)-models). Bianchi type I and IX can even be constrained to isotropic metrics, i.e. $F \cong SU(2)$. (The only other class A model for which this is possible is type VII₀. It yields, however, an isotropic model equivalent to that of type I [27].) These two models will be most interesting in the following, because we can successively increase the symmetry and observe properties of the quantum symmetry reduction step by step. The essential idea of the quantum symmetry reduction of [20] is to pull back a function on the unconstrained space of connections to a function on the space of invariant connections by means of the reconstruction map (1). For the models considered here the pull-back can be decomposed into a map which

leads to a function on the space of homogeneous, but in general anisotropic, connections (this is the quantum symmetry reduction for Bianchi models) followed by a map which restricts the support of a function on the space of homogeneous connections to only rotationally invariant ones. The second map, which can be viewed as a symmetry reduction of its own, provides us with a good test place for some of the ideas of quantum symmetry reduction.

These models with enhanced symmetry can be treated on an equal footing by writing the symmetry group as the semidirect product $S = N \rtimes_{\rho} F$, with the isotropy subgroup F and the translational subgroup N, which is one of the Bianchi groups. The composition in this group is defined as $(n_1, f_1)(n_2, f_2) := (n_1\rho(f_1)(n_2), f_1f_2)$ which depends on the group homomorphism $\rho: F \to \operatorname{Aut} N$ into the automorphism group of N (which for ease of notation will be denoted by the same letter as the representation on $\operatorname{Aut} \mathcal{L}N$ used below). Inverse elements are given by $(n, f)^{-1} = (\rho(f^{-1})(n^{-1}), f^{-1})$. To determine the form of invariant connections we have to calculate the Maurer–Cartan form on S (using the usual notation):

$$\begin{split} \theta_{\text{MC}}^{(S)}(n, f) &= (n, f)^{-1} \mathsf{d}(n, f) \\ &= (\rho(f^{-1})(n^{-1}), f^{-1})(\mathsf{d}n, \mathsf{d}f) \\ &= (\rho(f^{-1})(n^{-1})\rho(f^{-1})(\mathsf{d}n), f^{-1} \mathsf{d}f) \\ &= (\rho(f^{-1})(n^{-1} \mathsf{d}n), f^{-1} \mathsf{d}f) \\ &= (\rho(f^{-1})(\theta_{\text{MC}}^{(N)}(n)), \theta_{\text{MC}}^{(F)}(f)) \,. \end{split}$$

Here the Maurer–Cartan forms $\theta_{\text{MC}}^{(N)}$ on N and $\theta_{\text{MC}}^{(F)}$ on F appear. We next have to choose an embedding $\iota: S/F = N \hookrightarrow S$, which can most easily be done as $\iota: n \mapsto (n, 1)$. We then have $\iota^*\theta_{\text{MC}}^{(S)} = \theta_{\text{MC}}^{(N)}$, and a reconstructed connection takes the form $\phi \circ \iota^*\theta_{\text{MC}}^{(S)} = \phi_I^i \omega^I \tau_i$ which is the same as for anisotropic models of the last subsection (where now ω^I are left invariant 1-forms on the translation group N). However, here ϕ is constrained by equation (2) and we only get a subset as isotropic connections.

To solve the Higgs equation we have to treat LRS and isotropic models separately. In the first case we choose $\mathcal{L}F = \langle \tau_3 \rangle$, whereas in the second case we have $\mathcal{L}F = \langle \tau_1, \tau_2, \tau_3 \rangle$ ($\langle \cdot \rangle$ denotes the linear span). Equation (2) can be written infinitesimally as

$$\phi(\operatorname{ad}_{\tau_i}(T_I)) = \operatorname{ad}_{\operatorname{d}\lambda(\tau_i)}\phi(T_I) = [\operatorname{d}\lambda(\tau_i), \phi(T_I)]$$

(i=3 for LRS, $1 \le i \le 3$ for isotropy). The T_I denote the generators of $\mathcal{L}N = \mathcal{L}F_{\perp}$, on which the isotropy subgroup F acts as rotation: $\mathrm{ad}_{\tau_i}(T_I) = \epsilon_{iIK}T_K$. This is the derivative of the representation ρ defining the semidirect product S. The conjugation on the left-hand side of the Higgs equation (2) is

$$Ad_{(1,f)}(n, 1) = (1, f)(n, 1)(1, f^{-1}) = (\rho(f)(n), 1),$$

which follows from the composition in S.

We next have to determine the possible conjugacy classes of homomorphisms $\lambda: F \to G$. For LRS models their representatives are given by

$$\lambda_k: U(1) \to SU(2), \exp(t\tau_3) \mapsto \exp(kt\tau_3)$$
 for $k \in \mathbb{N}_0 = \{0, 1, \ldots\}$

(for a derivation see the example of spherical symmetry in [20] which is in many respects similar to LRS models). Choosing these representatives for $[\lambda_k]$ will be called τ_3 -gauge. For the components ϕ_I^i of ϕ defined by $\phi(T_I) = \phi_I^i \tau_i$ the Higgs equation takes the form $\epsilon_{3IK}\phi_K^j = k\epsilon_{3lj}\phi_I^l$. This can be written as a matrix equation $E_3\Phi = k\Phi E_3$ with $(E_3)_{ij} := \epsilon_{3ij}$ and $(\Phi)_{ij} := \phi_i^j$ (indeed the Higgs equation can be interpreted as an equation for ϕ to be an intertwiner between certain subrepresentations of the representation of F on $\mathcal{L}F_\perp$ and the

adjoint representation of G [32]). This equation has a non-trivial solution only for k = 1, in which case ϕ can be written as

$$\phi_1 = 2^{-\frac{1}{2}}(a\tau_1 + b\tau_2), \qquad \phi_2 = 2^{-\frac{1}{2}}(-b\tau_1 + a\tau_2), \qquad \phi_3 = c\tau_3$$

with arbitrary numbers a, b, c (the factors of $2^{-\frac{1}{2}}$ are introduced for the sake of normalization). The conjugate momenta take the form

$$p^{1} = 2^{-\frac{1}{2}}(p_{a}\tau_{1} + p_{b}\tau_{2}), \qquad p^{2} = 2^{-\frac{1}{2}}(-p_{b}\tau_{1} + p_{a}\tau_{2}), \qquad p^{3} = p_{c}\tau_{3}.$$

The symplectic structure is given by

$${a, p_a} = {b, p_b} = {c, p_c} = \kappa \iota'$$

and vanishes in all other cases.

In the case of isotropic models we have only the two homomorphisms $\lambda_0: SU(2) \to SU(2)$, $f \mapsto 1$ and $\lambda_1 = \mathrm{id}$ (again, this will be called τ_3 -gauge; for ease of notation we use the same letters for the homomorphisms as in the LRS case, which is justified by the fact that the LRS homomorphisms are restrictions of those appearing here). The Higgs equation takes the form $\epsilon_{iIK}\phi_K^j = 0$ for λ_0 with no non-trivial solution, and $\epsilon_{iIK}\phi_K^j = \epsilon_{ilj}\phi_I^l$. Each of the last equations has the same form as for LRS models with k=1, and their solution is $\phi_I^i = c\delta_I^i$ with an arbitrary c. In this case the conjugate momenta can be written as $p_i^l = p\delta_i^l$, and we have the symplectic structure $\{c, p\} = \kappa t'$.

Thus, we see that in both cases there is a unique non-trivial sector, and no topological charge appears.

To be more concrete, we now calculate the form of metric tensors for Bianchi I and IX, and its related isotropic models. Because we have the dreibein components e_I^i , which represent the inverse matrix of p_i^I , line elements are given by $\mathrm{d}s^2 = e_I^i e_{iJ} \omega^I \otimes \omega^J$. Thus we have to calculate the left invariant 1-forms on \mathbb{R}^3 for Bianchi I, and on SU(2) for Bianchi IX. For Bianchi I we clearly have $\omega^I = \mathrm{d}x^I$ in a coordinate system adapted to the translational symmetry. The line element is $\mathrm{d}s^2 = e_I^i e_{iJ} \mathrm{d}x^I \otimes \mathrm{d}x^J$, and in case of isotropy, i.e. $e_I^i = e\delta_I^i$, $\mathrm{d}s^2 = e^2[(\mathrm{d}x^1)^2 + (\mathrm{d}x^2)^2 + (\mathrm{d}x^3)^2]$, which is the metric of an isotropic flat universe.

For Bianchi IX, i.e. for the translational symmetry group SU(2), the left invariant 1-forms can be calculated, e.g. by using the parameterization $g = \exp(2rn^i\tau_i) \in SU(2)$ with $0 \le r < 2\pi$ and $n = (\sin \vartheta \cos \varphi, \sin \vartheta \sin \varphi, \cos \vartheta)$, from $g^{-1}dg = \omega^I \tau_I$:

$$\omega^{1} = 2\sin\vartheta\cos\varphi\,dr + [\sin 2r\cos\vartheta\cos\varphi - (\cos 2r - 1)\sin\varphi]\,d\vartheta$$
$$+ [-\sin 2r\sin\vartheta\sin\varphi - (\cos 2r - 1)\sin\vartheta\cos\vartheta\cos\varphi]\,d\varphi$$
$$\omega^{2} = 2\sin\vartheta\sin\varphi\,dr + [\sin 2r\cos\vartheta\sin\varphi + (\cos 2r - 1)\cos\varphi]\,d\vartheta$$
$$+ [\sin 2r\sin\vartheta\cos\varphi - (\cos 2r - 1)\sin\vartheta\cos\vartheta\sin\varphi]\,d\varphi$$

$$\omega^{3} = 2\cos\vartheta \,dr - \sin 2r\sin\vartheta \,d\vartheta + (\cos 2r - 1)\sin^{2}\vartheta \,d\varphi.$$

In the isotropic case we obtain the metric

$$ds^2 = e^2 \sum_{I=1}^3 \omega^I \otimes \omega^I = 4e^2 [(dr)^2 + \sin^2 r \, d\Omega^2]$$

of an isotropic closed model of positive spatial curvature.

Finally, we have to specialize the constraints derived in the preceding subsection to the enhanced symmetry. To that end we first relax the partial gauge fixing introduced above by choosing the representative λ_1 . In general we can choose any homomorphism out of its conjugacy class, i.e. λ_1 can be replaced by $g^{-1}\lambda_1 g$ for any $g \in G = SU(2)$. For the LRS

models this amounts to replacing τ_i in the expressions for ϕ_I by $g^{-1}\tau_i g =: \Lambda_i^j \tau_j$. Thus, we obtain

$$\phi_1^i = 2^{-\frac{1}{2}} (a\Lambda_1^i + b\Lambda_2^i), \qquad \phi_2^i = 2^{-\frac{1}{2}} (-b\Lambda_1^i + a\Lambda_2^i), \qquad \phi_3^i = c\Lambda_3^i$$

and analogously for p_i^I . The matrix Λ fulfils the relations $\Lambda_i^k \Lambda_k^j = \delta_i^j$ and $\epsilon_{ijk} \Lambda_l^i \Lambda_m^j \Lambda_n^k = \epsilon_{lmn}$, which can be derived by calculating $\operatorname{tr}(g^{-1}\tau_i g g^{-1}\tau^j g)$ and $\operatorname{tr}(g^{-1}\tau_l g g^{-1}\tau_m g g^{-1}\tau_n g)$, respectively. The expressions for isotropic models can be obtained by setting b = 0 and $a = \sqrt{2}c$.

The Gauß constraint now takes the form

$$\mathcal{G}^{i} = (\kappa \iota')^{-1} \epsilon_{ijk} \left[c p_{c} \Lambda_{3}^{j} \Lambda_{3}^{k} + \frac{1}{2} (a \Lambda_{1}^{j} + b \Lambda_{2}^{j}) (p_{a} \Lambda_{1}^{k} + p_{b} \Lambda_{2}^{k}) \right. \\
\left. + \frac{1}{2} (-b \Lambda_{1}^{j} + a \Lambda_{2}^{j}) (-p_{b} \Lambda_{1}^{k} + p_{a} \Lambda_{2}^{k}) \right] \\
= (\kappa \iota')^{-1} (a p_{b} - b p_{a}) \Lambda_{3}^{i} .$$
(9)

To simplify the diffeomorphism constraint we use the fact that for class A models the structure constants can be written as $c_{IJ}^K = \epsilon_{IJL} n^{LK}$ with a symmetric matrix n^{LK} which can be diagonalized to $n^{LK} = n^{(K)} \delta^{LK}$ with eigenvalues $n^{(K)}$. The (dedensitized) constraint then becomes

$$\mathcal{D}_a N^a = -(2\kappa \iota')^{-1} N^3 (-c_{32}^1 + c_{31}^2) (ap_b - bp_a)$$

= $-\frac{1}{2} (n^{(1)} + n^{(2)}) (\kappa \iota')^{-1} N^3 (ap_b - bp_a)$, (10)

which already vanishes if the Gauß constraint is solved. This is a consequence of an interrelation of SU(2)-gauge transformations and diffeomorphisms due to the Higgs constraint which will be explained in more detail when quantizing the constraints.

The Euclidean part of the dedensitized Hamiltonian constraint is

$$g_0^{-1}\mathcal{H}^{(E)} = -(n^{(1)} + n^{(2)})(ap_a + bp_b)p_c - n^{(3)}c(p_a^2 + p_b^2) + (ap_a + bp_b + cp_c)^2 - \frac{1}{2}(ap_a + bp_b)^2 - (cp_c)^2 + \frac{1}{2}(ap_b - bp_a)^2.$$
 (11)

For isotropic models (a = b = c, $p_a = p_b = p_c =: p$) the constraints \mathcal{G}^i and \mathcal{D}_a vanish identically, whereas the Euclidean part of the Hamiltonian constraint takes the form

$$g_0^{-1}\mathcal{H}^{(E)} = -2(n^{(1)} + n^{(2)} + n^{(3)})cp^2 + 6(cp)^2$$
(12)

where $n^{(1)} = n^{(2)} = n^{(3)} = 0$ for isotropic flat (Bianchi I), and $n^{(1)} = n^{(2)} = n^{(3)} = 1$ for isotropic closed (Bianchi IX).

3.3. Auxiliary Hilbert spaces for homogeneous models

The configuration spaces for our models are given by Higgs 'fields' in a single point, which shows that they are finite-dimensional. In quantum theory they will be represented as spaces of point holonomies [23] associated with a single point, the only point x_0 in the reduced manifold B. For the anisotropic models with an empty Higgs condition (2) there are three independent SU(2)-Higgs fields, ϕ_1 , ϕ_2 and ϕ_3 , associated with the independent directions T_I in the tangent space of x_0 . Thus, we have three point holonomies $h_I := \exp \phi_I^i \tau_i$ lying in a single vertex (the point x_0), in which SU(2)-gauge invariance has to be imposed. The auxiliary Hilbert space on which the constraints have to be solved is the space $\mathcal{H}_{\text{aux}} = L^2([SU(2)]^3, [d\mu_H]^3)$ of functions of the three point holonomies. Its measure is analogous to the Ashtekar–Lewandowski measure $(d\mu_H)$ is the Haar measure on SU(2)). The momenta p_I^I will be represented as derivative operators on functions in \mathcal{H}_{aux} . To calculate their action we need the small

Lemma 1. Let G be a Lie group and $F: \mathbb{R} \to \mathcal{L}G$ be a differentiable $\mathcal{L}G$ -valued function in a real parameter. The derivative of $\exp F(s) \in G$ with respect to s in the point $s = s_0$ is given by

$$\frac{\mathrm{d} \exp F(s)}{\mathrm{d} s} \bigg|_{s=s_0} = \int_0^1 \mathrm{d} t \exp(tF(s_0)) F'(s_0) \exp[(1-t)F(s_0)]$$

where F' is the derivative of F with respect to s.

Proof. The derivative

$$\frac{\operatorname{d} \exp F(s)}{\operatorname{d} s} \bigg|_{s=s_0} := \lim_{s \to s_0} \frac{\exp F(s) - \exp F(s_0)}{s - s_0}$$

$$= \lim_{s \to s_0} \frac{\exp F(s) \exp(-F(s_0)) - 1}{s - s_0} \exp F(s_0)$$

can be written as

$$\begin{split} \frac{\mathrm{d} \exp F(s)}{\mathrm{d} s} \bigg|_{s=s_0} &= \lim_{s \to s_0} (s-s_0)^{-1} \int_0^1 \mathrm{d} t \, \frac{\mathrm{d}}{\mathrm{d} t} [\exp(tF(s)) \exp(-tF(s_0))] \exp F(s_0) \\ &= \lim_{s \to s_0} \int_0^1 \mathrm{d} t \exp(tF(s)) \frac{F(s) - F(s_0)}{s - s_0} \exp(-tF(s_0)) \exp F(s_0) \\ &= \int_0^1 \mathrm{d} t \exp(tF(s_0)) F'(s_0) \exp[(1-t)F(s_0)] \, . \end{split}$$

Applied to $\exp \phi_I^i \tau_i$ we get for the action of $\frac{\partial}{\partial \phi_J^i}$

$$\frac{\partial}{\partial \phi_J^i} \exp(\phi_I^i \tau_i) = \delta_I^J \int_0^1 \mathrm{d}t \exp(t \phi_I^i \tau_i) \tau_j \exp[(1-t) \phi_I^i \tau_i]$$

which cannot be represented as an element of the auxiliary Hilbert space (it contains a continuous family of point holonomies). Analogously to [23] we can regularize the Higgs vertex by smearing the point holonomy to a holonomy associated with a regularizing edge. This introduces a δ -function into the action of $\frac{\partial}{\partial \phi_I^t}$ which is non-vanishing only in the endpoints of the edge corresponding to t=0 and t=1 in the formula of the lemma, and the momenta get quantized to combinations of left and right invariant vector fields

$$\hat{p}_{i}^{I} = -i\iota' l_{P}^{2} \sum_{J=1}^{3} \frac{\partial (h_{J})_{B}^{A}}{\partial \phi_{I}^{i}(x_{0})} \frac{\partial}{\partial (h_{J})_{B}^{A}}
= -i\iota' l_{P}^{2} \sum_{J=1}^{3} \frac{1}{2} (\tau_{i} h_{I} + h_{I} \tau_{i})_{B}^{A} \frac{\partial}{\partial (h_{I})_{B}^{A}}
= -\frac{1}{2} i\iota' l_{P}^{2} \left(X_{i}^{(L)}(h_{I}) + X_{i}^{(R)}(h_{I}) \right)$$
(13)

acting on the Ith copy of SU(2) in the domain of definition of a function in \mathcal{H}_{aux} (the δ -function is integrated to $\frac{1}{2}$ because its singularity lies at the endpoints of the domain of integration).

Of course, in B there is no place for a regularizing edge. Therefore, we introduce a compact auxiliary manifold homeomorphic to $\overline{S/F}$. The bar reminds us that we may have to take a certain compactification (e.g. the one-point compactification of \mathbb{R}^3 for Bianchi I) of S/F (this is not necessary for Bianchi IX), and we take into account the possibility of a non-trivial isotropy subgroup F for later use. We need this space only as a differentiable manifold: the

group structure of S does not play any role here. On S/F we have the vector fields X_I dual to the left invariant 1-forms ω^I used earlier. With their help we define curves e_I : $[0, 1] \to \overline{S/F}$ by the differential equation $\dot{e}_I(t) = X_I(e_I(t))$, and we assume the compactification of S/F to be taken in such a way that the three curves e_I are closed. We take them as regularizing edges for the three-point holonomies, which is justified by the equation

$$h(e_I) := \mathcal{P} \exp \int_0^1 \mathrm{d}t \, \dot{e}_I^a A_a^i \tau_i = \mathcal{P} \exp \int_0^1 \mathrm{d}t \, \phi_J^i \, \omega^J(\dot{e}_I) \tau_i = \exp(\phi_I^i \tau_i)$$

for the holonomy along e_I of a reconstructed connection on $\overline{S/F}$. The auxiliary Hilbert space is then generated by spin network states associated with graphs consisting of the three closed edges e_I , which meet in the 6-vertex x_0 , and which are labelled by spins $j_I \in \frac{1}{2}\mathbb{N}_0$. There is some arbitrariness in the directions of the e_I : depending on the special model there is gauge freedom due to the diffeomorphism constraint which acts by inner automorphisms of S. This freedom will be fixed by solving the diffeomorphism constraint in section 5; for the moment we can choose some appropriate directions for the e_I which amounts to a total gauge fixing of reduced diffeomorphisms.

For a non-trivial isotropy subgroup F the situation is more complicated. At first, classically the gauge is fixed partially: for LRS models the reduced gauge group is U(1), whereas for isotropic models it is fixed totally and there is no gauge group at all. These facts are nicely illustrated by the Gauß constraint for these models, which is proportional to Λ_3^i , and which forms the internal axis of the remaining gauge freedom for LRS models with gauge fixing given by Λ , or vanishes completely in the case of isotropic models. In the quantum theory the partial gauge fixing can (and has to) be undone (here lies the advantage of the general framework described in section 2). Thus, we will use SU(2)-holonomies also for LRS and isotropic models.

In addition, one has the Higgs equation (2) to be solved. By exponentiating, it can be written as

$$h(f(e_I)) := \exp \phi(\operatorname{Ad}_f(T_I))$$

$$= \exp \operatorname{Ad}_{\lambda(f)} \phi(T_I)$$

$$= \operatorname{Ad}_{\lambda(f)} \exp \phi(T_I)$$

$$= \operatorname{Ad}_{\lambda(f)} h(e_I)$$
(14)

and interpreted as a condition for holonomies which are obtained by rotating the edges e_I . As a first application of this equation, which provides a geometrical interpretation of the Higgs constraint, one can easily see that usage of the homomorphism λ_0 does not lead to a non-vanishing Higgs field: the right-hand side is then identically $h(e_I)$, whereas for f, a rotation by 180° , the left-hand side becomes $h(e_I)^{-1}$. The equation can be fulfilled only for $h(e_I) = 1$, i.e. a vanishing Higgs field. This consideration can be extended to all even values of k. Furthermore, we see that rotated holonomies are gauge equivalent and therefore some of them are redundant. Roughly, this leads to only two independent holonomies for LRS models (an axial one $h(e_3)$, which we choose in the 3-direction, and a transversal one $h(e_1)$ representing the two equivalent holonomies), and only one for isotropic models. However, there are subtleties because of the twisting introduced by gauge rotations on the right-hand side of equation (14). To make it clear we first treat the λ_0 -sectors pretending, for illustrative purposes only, that they would lead to non-trivial Higgs fields.

For anisotropic models the classical configuration space is given by $\mathcal{U}=SU(2)^3=\{(\exp(\phi_1^i\tau_i),\exp(\phi_2^i\tau_i),\exp(\phi_3^i\tau_i))\}$. Equation (14) then states that all three holonomies are the same for an isotropic model, i.e. in this case we have the configuration space $\mathcal{U}_{\rm iso}^{[\lambda_0]}=\{(h,h,h):h\in SU(2)\}$, which is the diagonal SU(2)-subgroup of $SU(2)^3$. This

is the would-be solution space of the Higgs condition leading to the auxiliary Hilbert space $L^2(SU(2), d\mu_H)$ spanned by spin networks associated with graphs consisting of a single closed edge. In the case of LRS models this consideration leads to two independent holonomies. But the situation described in the present paragraph does not appear, because for λ_0 we have no non-trivial Higgs field. Therefore, we have to determine the classical configuration space for the realistic λ_1 -sectors with their twisting in equation (14).

For LRS models in the τ_3 -gauge, we have again a subspace of $SU(2)^3$ parameterized by the parameters $a =: A \cos \alpha$, $b =: A \sin \alpha$, c introduced above as

$$\mathcal{U}_{LRS}^{\tau_3} = \{ (\exp(A \, n^i(\alpha) \tau_i), \exp(A \, \epsilon_{3ij} n^i(\alpha) \tau^j), \exp(c \tau_3)) \}$$

with $n^i = (\cos \alpha, \sin \alpha, 0)$. The parameter α is pure gauge, whereas the parameters A, c represent the gauge-invariant information. The configuration space on which the partial gauge fixing is undone is the union of the conjugacy classes of all elements of $\mathcal{U}_{LRS}^{\tau_3}$. It can be written as

$$\mathcal{U}_{LRS}^{[\lambda_1]} = \{ (\exp(A\Lambda_1^i \tau_i), \exp(A\Lambda_2^i \tau_i), \exp(c\Lambda_3^i \tau_i)) \}$$
 (15)

and depends only on the conjugacy class $[\lambda_1]$. It is parameterized by five parameters: A, c, and the three angles which determine the dreibein Λ^i_j . For isotropic models we can obtain $\mathcal{U}^{[\lambda_1]}_{\mathrm{iso}}$ by setting A=c.

Going over from \mathcal{U}^{τ_3} to $\mathcal{U}^{[\lambda_1]}$ introduces no new degrees of freedom as long as we require functions on $\mathcal{U}^{[\lambda_1]}$ to be gauge invariant under diagonal SU(2)-conjugation. This restores the original gauge group SU(2) of the non-symmetric theory. Our reason for doing so is twofold: first, the partial gauge fixing is undone, and the reduced theory will only depend on $[\lambda_1]$, not on the selection of a representative. Second, we will be able to use techniques developed for SU(2)-spin networks, which would not be possible in the gauge-fixed case.

Now we can see the difference between the fake λ_0 -case above and the realistic λ_1 -case: for λ_0 the solution space of the Higgs equation was a subgroup of $SU(2)^3$. Thus we could use the Peter-Weyl theorem to identify all functions on this manifold with matrix elements of SU(2)-representations, which lead us to spin networks associated with a reduced number of edges. However, due to the twisting for λ_1 the solution space is no longer a subgroup, but only a union of conjugacy classes in $SU(2)^3$. The Peter-Weyl theorem no longer applies, and we have to determine all functions on $\mathcal{U}^{[\lambda_1]}$ by hand. Of course, the spin network states with a reduced number of edges are some of those functions. For example, for isotropic models they can be obtained from spin networks in the anisotropic theory with two of the three labellings being zero. But these do not comprise all functions on $\mathcal{U}^{[\lambda_1]}_{iso}$ one can easily see that all such gauge-invariant spin network functions with one edge are symmetric under $c\mapsto -c$ if they are evaluated in $h=\exp(c\Lambda_3)$. But there are gauge-invariant functions on $\mathcal{U}^{[\lambda]}_{iso}$ which are not symmetric under this reflection: one example is given by $\operatorname{tr}[\exp(c\Lambda_1)\exp(c\Lambda_2)\exp(c\Lambda_3)]=2\cos^3(c/2)-2\sin^3(c/2)$, which stems from an anisotropic spin network with all labellings being $\frac{1}{2}$ and an appropriate vertex contractor. The situation for LRS models is similar: ordinary spin networks with two edges do not suffice.

Thus there are more gauge-invariant functions on the classical configuration space than naively expected. We will discuss this in more detail and derive all such functions in the second part [24]. Regarding the purposes of the present part, i.e. quantization and solution of Gauß and diffeomorphism constraints, no important new features are introduced by these additional functions. At this stage it suffices to know that all such functions can be viewed as spin network functions with two (LRS) or one (isotropic) edge, but possibly with a certain insertion in the vertex x_0 (for isotropic models the auxiliary Hilbert space is doubled in this way) which neither affects the action of gauge transformations nor of diffeomorphisms. This

insertion can be viewed as a reduction of the vertex contractor in spin networks with three closed edges, which was not taken into account in the naive arguments presented above.

4. Gauß constraints

We proceed now by quantizing the Gauß constraint (5) on the auxiliary Hilbert space derived in the preceding section. To that end we introduce new parameters which substitute the Higgs field components ϕ_I^i and which are better suited for this purpose. These new coordinates r_I , α_I^3 , β_I^3 are, independently for each $1 \le I \le 3$, defined by $\phi_I^i =: r_I n_3^i(\alpha_I^3, \beta_I^3)$ with $n_3^i(\alpha, \beta) := (\cos \alpha \sin \beta, \sin \alpha \sin \beta, \cos \beta)$. Alternatively, we can choose the parameters α_I^2 , β_I^2 defined analogously with $n_2^i(\alpha, \beta) := (\sin \alpha \sin \beta, \cos \beta, \cos \alpha \sin \beta)$, or the parameters α_I^1 , β_I^1 with $n_1^i(\alpha, \beta) := (\cos \beta, \cos \alpha \sin \beta, \sin \alpha \sin \beta)$. It is easy to see that these new parameters fulfil

$$\frac{\partial}{\partial \alpha_I^i} = \epsilon_{ijk} \phi_I^j \frac{\partial}{\partial \phi_I^k} \qquad \text{(no sum over } I).$$

Thus, we can quantize the Gauß constraint (5) acting on a function $f \in \mathcal{H}_{aux}$ as

$$\hat{\mathcal{G}}_{i}f = \frac{\hbar}{\mathrm{i}} \epsilon_{ijk} \phi_{I}^{i} \frac{\partial f}{\partial \phi_{I}^{k}} = \frac{\hbar}{\mathrm{i}} \sum_{I=1}^{3} \frac{\partial f}{\partial \alpha_{I}^{i}}$$

where we use either of the three sets of angular parameters depending on the component of the Gauß constraint.

To calculate the derivative we note that a point holonomy

$$h_I = \exp(\phi_I^i \tau_i) = \exp(r_I n_3^i (\alpha_I^3, \beta_I^3) \tau_i)$$

gets changed under a gauge transformation with $\exp(\gamma \tau_3)$ into

$$\exp(\gamma \tau_3) \exp(r_I n_3^i(\alpha_I^3, \beta_I^3) \tau_i) \exp(-\gamma \tau_3) = \exp(r_I n_3^i(\alpha_I^3 + \gamma, \beta_I^3) \tau_i).$$

Thus g_I can be written as $h_I = \exp(\alpha_I^3 \tau_3) \exp(r_I n_3^i(0, \beta_I^3) \tau_i) \exp(-\alpha_I^3 \tau_3)$, and analogously for α_I^2 or α_I^1 . The derivative of h_I with respect to α_I^i can now be calculated as

$$\frac{\partial h_I}{\partial \alpha_I^i} = \tau_i h_I - h_I \tau_i .$$

With this relation the Gauß constraint acting on the function $f(h_1, h_2, h_3)$ becomes

$$\begin{split} \hat{\mathcal{G}}_{i}f &= \frac{\hbar}{\mathrm{i}} \sum_{I=1}^{3} \frac{\partial f}{\partial \alpha_{I}^{i}} \\ &= \frac{\hbar}{\mathrm{i}} \sum_{I=1}^{3} \left(\frac{\partial (h_{I})_{B}^{A}}{\partial \alpha_{I}^{i}} \right) \frac{\partial f}{\partial (h_{I})_{B}^{A}} \\ &= \frac{\hbar}{\mathrm{i}} \sum_{I=1}^{3} (\tau_{i}h_{I} - h_{I}\tau_{i})_{B}^{A} \frac{\partial f}{\partial (h_{I})_{B}^{A}} \\ &= \frac{\hbar}{\mathrm{i}} \sum_{I=1}^{3} \left(X_{i}^{(R)}(h_{I}) - X_{i}^{(L)}(h_{I}) \right) f \end{split}$$

with the difference of a right and left invariant vector field for each point holonomy. This action is as expected, because each of the point holonomies transforms with respect to the adjoint representation under a gauge transformation.

The solution of the constraint can be given in a standard way by restricting the Hilbert space to the gauge-invariant subspace spanned by gauge-invariant spin network states, i.e.

those spin networks whose intertwiner in the vertex x_0 contracts the six representations (an incoming and an outgoing for each of the three edges) to the trivial representation.

For LRS models we have to quantize the reduced constraint (9). After introducing the angle $\alpha := \arctan b/a$ it can, analogously to the calculations above, be written as

$$\hat{\mathcal{G}}_{i} f = \frac{\hbar}{i} \Lambda_{3}^{i} \Lambda_{3}^{j} \left(X_{j}^{(R)}(h_{1}) - X_{j}^{(L)}(h_{1}) \right) f.$$

Note that after solving the Higgs constraint a function f in the auxiliary Hilbert space only depends on the two point holonomies $h_1 = \exp(a\Lambda_1^i + b\Lambda_2^i)\tau_i$ and $h_3 = \exp(c\Lambda_3^i\tau_i)$.

There are two points to mention about this operator. First, classically Λ_i^3 is fixed so that the quantization of the Gauß constraint consists of only one component of invariant vector fields (X_3) in the τ_3 -gauge), and it would force only this component to vanish if we would use this partial gauge fixing in quantum theory. This corresponds to the fact that the reduced structure group for F = U(1) is U(1) consisting of internal rotations around an axis determined by the partial gauge fixing Λ_3^i . However, we have already relaxed the partial gauge fixing to arrive at our auxiliary Hilbert space. In this process, functions on the partially gauge-fixed configuration space $\mathcal{U}_{LRS}^{\tau_3}$ can be extended to functions on $\mathcal{U}_{LRS}^{[\lambda_1]}$ by demanding invariance under conjugation. Only for those functions can the gauge-fixed Gauß constraint be used. On an arbitrary function on $\mathcal{U}_{LRS}^{[\lambda_1]}$ we have to impose all three components of an SU(2)-constraint. (For a similar discussion in the case of spherically symmetric quantum gravity see [20].)

Second, the operator contains only vector fields associated with the holonomy h_1 , whereas the axial holonomy h_3 does not appear at all. At first one would expect both holonomies to contribute equally, because the auxiliary Hilbert space is spanned by spin network states with the two edges e_1 and e_3 meeting in the vertex x_0 . But after taking into account the construction of the solution space $\mathcal{U}_{LRS}^{[\lambda_1]}$ of the Higgs equation, vanishing of the e_3 -contribution is completely consistent: the Gauss constraint contains the Λ_3^i -component of vector fields, and due to $h_3 = \exp(c\Lambda_3^i\tau_i)$ on $\mathcal{U}_{LRS}^{[\lambda_1]}$ (Λ is now a coordinate on that space) we have

$$\Lambda_3^i X_i^{(R)}(h_3) = \operatorname{tr} \left[(\Lambda_3^i \tau_i h_3)^T \frac{\partial}{\partial h_3} \right] = \operatorname{tr} \left[(h_3 \Lambda_3^i \tau_i)^T \frac{\partial}{\partial h_3} \right] = \Lambda_3^i X_i^{(L)}(h_3).$$

Thus, the Λ_3^i -components of the right and left invariant vector fields are the same, and they cancel one another in the Gauß constraint. Therefore, they do not appear any more in the partially fixed Gauß constraint acting on functions on $\mathcal{U}_{LRS}^{[\lambda_1]}$.

After this discussion we see that the Gauß constraint can be solved in the quantum theory, without partial gauge fixing, by gauge-invariant SU(2)-spin networks. Here, only two edges meet in the 4-vertex x_0 (the insertion mentioned in the preceding section does not affect this consideration).

Having the discussion of LRS models in mind we can treat the isotropic briefly. Classically, the gauge group is completely broken, $Z_G(\lambda_1(F)) = \{1\}$, and one would not expect a Gauß constraint. However, in quantum theory, after undoing the gauge fixing we use SU(2)-spin networks with a single edge, which should be gauge invariant in the vertex x_0 , i.e. the two copies of the representation to the label j, one for the incoming and one for the outgoing part of the closed edge, should be contracted to the trivial representation in x_0 .

5. Diffeomorphism constraints

Before quantizing the diffeomorphism constraint we briefly describe the role played by diffeomorphisms in symmetry-reduced models. By using ansätze for invariant fields adapted to the symmetry, some freedom in applying diffeomorphisms is fixed. Classically, this arises

because one uses special coordinates which exhibit the symmetry, e.g. polar coordinates in the case of spherical symmetry. Therefore, only diffeomorphisms respecting the ansätze are realized in the symmetry-reduced theory. These are typically diffeomorphisms of the reduced manifold B, e.g. a radial manifold in case of spherical symmetry, whereas the remaining freedom is fixed. But for the homogeneous models studied here the reduced manifold $B = \{x_0\}$ consists of a single point, and one may ask why the diffeomorphism constraint (7) does not vanish, for there are now no diffeomorphisms of the reduced manifold.

A hint at an answer to that question comes from the fact that (7) generates inner automorphisms of the symmetry group S, the group manifold of which is identified (modulo compactification) with the homogeneous space manifold Σ . This can be seen from the fact that the expression (7) is similar to the constraint (5), which generates conjugation in the internal space, except for an exchange of the structure constants ϵ_{ijk} of SU(2) with the ones c_{IJ}^K of S.

The remaining freedom after choosing coordinates adapted to the symmetry is to select an origin x_0 of the coordinate system. Instead of x_0 we could choose any other point sx_0 , $s \in S$ in Σ (we can indeed reach any other point owing to transitivity of the group action). Using the base point x_0 , all points gx_0 in Σ can be parameterized by the group coordinates of g (this group element is unique if there is no isotropy subgroup, otherwise we can use coordinates of gF_{x_0} in the homogeneous space S/F_{x_0}). But after performing a left translation with s, which shifts the origin to sx_0 , the point gx_0 is mapped to $sgx_0 = (sgs^{-1})sx_0$. Thus, upon changing the base point, the role of S (providing coordinates on Σ) is played by the isomorphic group sSs^{-1} . Inner automorphisms of S are the remaining gauge freedom under the diffeomorphism group, and the diffeomorphism constraint—which demands independence of the physical phase space under inner automorphisms—can be seen to enforce independence of the selection of a base point. In the classically reduced manifold (consisting of a single point) these transformations have, of course, no geometric meaning. But in the course of quantization we introduced an auxiliary manifold when promoting point holonomies to holonomies associated with edges therein. The inner automorphisms act on this manifold and thereby move these edges depending on the symmetry group S. Strictly speaking, we have to relax the gauge fixing of the diffeomorphism group which we introduced implicitly earlier by fixing three edges in the auxiliary manifold on which a spin network function depends. To study the action of diffeomorphisms and to eventually solve the constraint, we have to allow spin networks associated to graphs with three edges which can be transformed against the original edges.

For example, for Bianchi I all inner automorphisms are trivial and there is no non-trivial action on the edges (the diffeomorphism constraint vanishes in this case), and for Bianchi IX the group of inner automorphisms is isomorphic to SO(3) rotating the three edges. The last example will be discussed below, because it will serve us to discuss the difference between gauge and symmetry. Note that the diffeomorphism group in this case acts identically to the additional symmetry group (F = SU(2)) imposed when constraining Bianchi IX to an isotropic model. But the treatment of gauge in the one case (by group averaging) and of symmetry in the other (by quantum symmetry reduction) is very different, as will be illustrated by this example.

5.1. Quantization

We now know the action which is generated by the diffeomorphism constraint, and we can use it to solve the constraint by group averaging. But for illustrative purposes we will first investigate whether the constraint can be quantized in its infinitesimal version. To that end we write the action of an inner automorphism generated by $T_K \in \mathcal{L}S$ on a point holonomy as

$$Ad(\exp(-\delta T_K)): S \to S, h \mapsto \exp(-\delta T_K)h \exp(\delta T_K)$$

with a parameter $\delta \in \mathbb{R}$. By differentiation, this determines a map on the Lie algebra of S: $Ad(exp(-\delta T_K))$: $\mathcal{L}S \to \mathcal{L}S$,

$$c^{I}T_{I} \mapsto \exp(-\delta T_{K})c^{I}T_{I} \exp(\delta T_{K}) = c^{I} \exp\left(\delta(c_{IK}^{J})_{I}^{J}\right)T_{J} =: c^{I} \operatorname{Ad}_{I}^{J}(\exp(-\delta T_{K}))T_{J}$$

where the matrix elements $\operatorname{Ad}_I^J(\exp(-\delta T_K))$ are defined in terms of the matrix exponential of the matrix $(c_{IK}^J)_I^J$.

Because the edges e_I : $[0, 1] \to \overline{S/F}$ are defined by direction T_I in the identity of S, they get transformed into

$$e_I(t) \mapsto e_I^{(\delta,K)}(t) := \exp(-\delta T_K) \exp(tT_I) \exp(\delta T_K),$$

 $\dot{e}_I^{(\delta,K)}(t) = \operatorname{Ad}_I^J(\exp(-\delta T_K))\dot{e}_J(t)$

which is an integral curve to the left invariant vector field $\operatorname{Ad}_I^J(\exp(-\delta T_K))X_J$. The holonomy along this new edge is

$$\begin{split} h(e_I^{(\delta,K)}) &= \mathcal{P} \exp \int_0^1 \mathrm{d}t \, \phi_J^i \omega^J (\mathrm{Ad}_I^L(\exp(-\delta T_K)) X_L) \tau_i \\ &= \mathcal{P} \exp \int_0^1 \mathrm{d}t \, \phi_L^i \, \mathrm{Ad}_I^L(\exp(-\delta T_K)) \tau_i \\ &= \mathcal{P} \exp \int_0^1 \mathrm{d}t \, \phi_L^i (\delta_I^L + \delta c_{IK}^L + O(\delta^2)) \tau_i = \exp[(\phi_I^i + \delta c_{IK}^L \phi_L^i + O(\delta^2)) \tau_i] \\ &= \exp(\phi_I^i \tau_i) + \delta \left. \frac{\mathrm{d}}{\mathrm{d}\delta} \right|_{\delta=0} \exp[(\phi_I^i + \delta c_{IK}^L \phi_L^i + O(\delta^2)) \tau_i] + O(\delta^2) \\ &= \exp(\phi_I^i \tau_i) + \delta c_{MK}^L \phi_L^j \frac{\partial}{\partial \phi_M^j} \exp(\phi_I^i \tau_i) + O(\delta^2) \end{split}$$

where we Taylor-expanded in δ . If we apply a function f to the transformed holonomy and again Taylor-expand, we obtain

$$\begin{split} f\left(h(e_I^{(\delta,K)})\right) - f\left(h(e_I)\right) &= f\left(\exp(\phi_I^i \tau_i) + \delta c_{MK}^L \phi_L^j \frac{\partial}{\partial \phi_M^j} \exp(\phi_I^i \tau_i) + O(\delta^2)\right) - f\left(\exp(\phi_I^i \tau_i)\right) \\ &= \delta c_{MK}^L \phi_L^j \frac{\partial h(e_I)_B^A}{\partial \phi_M^j} \frac{\partial}{\partial h(e_I)_B^A} f\left(h(e_I)\right) + O(\delta^2) \,. \end{split}$$

After replacing p_i^I by a functional derivative with respect to ϕ_I^i , in the course of quantization, the correct expression for a quantization of (7) is already provided. Up to $O(\delta^2)$ we obtain

$$\hat{\mathcal{D}}_K f = -i\hbar \delta^{-1} \left(f\left(h(e_1^{(\delta,K)}), h(e_2^{(\delta,K)}), h(e_3^{(\delta,K)}) \right) - f(h(e_1), h(e_2), h(e_3)) \right) + O(\delta^2)$$

where f depends on three holonomies $h(e_I)$, $1 \le I \le 3$. The component \mathcal{D}_K is defined by $\mathcal{D}_a N^a =: \mathcal{D}_K N^K$. We would get a quantization of the constraint if we could perform the limit $\delta \to 0$ in the last equation. In such a case the diffeomorphism constraint would just act as a Lie derivative. But we encounter here the same problem as for the diffeomorphism constraint in the full theory (appendix C of [33]): in the diffeomorphism-invariant Ashtekar–Lewandowski inner product the functions associated with a graph consisting of the edges e_I on the one hand and of the edges $e_I^{(\delta,K)}$ on the other are orthogonal for all $\delta \neq 0$, and the limit does not exist in the associated topology.

5.2. Group averaging

Instead of quantizing the infinitesimal constraint we can use the known action of diffeomorphisms on the auxiliary manifold to solve the constraint by group averaging [33]. This is a simple procedure because all graphs underlying cylindrical functions in the auxiliary Hilbert space have at most three edges. Generically, this will bring us back to the space of functions on holonomies to the three fixed edges used earlier. But graph symmetries have to be taken properly into account [33, 34], which will be done now for the example of Bianchi IX.

In this case the action generated by the diffeomorphism constraint consists of all rotations in the auxiliary manifold. Thus, it is the same as the action of the isotropy subgroup for an isotropic closed model. We will see how these different concepts of gauge and symmetry are implemented. To solve the diffeomorphism constraint by group averaging we first have to determine an allowed basis for the space of spin network states according to [34]. Allowed states are defined by summing over the index set of labels

$$\Xi(I) := \{ \xi : \text{there is a } \phi \in \text{Diff with } U(\phi)T_I = T_{\nu(I),\xi} \}$$

where I denotes a multi-label consisting of the graph $\gamma(I)$ and further labellings ξ for a spin network T_I . Diff is the diffeomorphism group, here SO(3), and U is its representation on the space of spin network functions. Furthermore, $n(I) := |\Xi(I)|$ is the number of elements of an orbit of the label I. An allowed basis is built from functions which are symmetric (this should not be confused with the symmetry group of the symmetry reduction) with respect to graph symmetries:

$$T_I^S := n(I)^{-\frac{1}{2}} \sum_{\xi \in \Xi(I)} T_{\gamma(I),\xi} ,$$

and their group averaging is

$$[T_I^S] := n(I)^{-\frac{1}{2}}[T_I] := n(I)^{-\frac{1}{2}} \sum_{\phi \in \text{Diff}} T_{\phi(I)}$$

which solves the diffeomorphism constraint. All other states of the allowed basis are annihilated by group averaging.

In the case of Bianchi IX all spin networks are associated with graphs consisting of three edges meeting in a 6-vertex which can all be obtained as rotations of a fixed dreibein. In general, spin network functions associated with graphs which are rotated against one another are orthogonal, the only exception being the case of graph symmetries. The group of graph symmetries is here the permutation group S_3 on the three edges. If we define the subgroup $\sigma(T) \leqslant S_3$ as the group of label symmetries which fix not only the graph but the whole labelling when acting on a spin network T, we can write the symmetric states of the allowed basis as

$$T^{S} = \sqrt{\frac{|\sigma(T)|}{|S_3|}} \sum_{\phi \in S_3/\sigma(T)} U(\phi)T.$$

There are three different cases: for $j_1=j_2=j_3$, i.e. identical labels for all three edges, we have $\sigma(T)=S_3$ and $T^S=T$. The case $j_1=j_2\neq j_3$ (and analogously $j_1\neq j_2=j_3$, $j_1=j_3\neq j_2$), $\sigma(T)\overset{\sim}{=}S_2$ leads to $T^S=3^{-\frac{1}{2}}(T+T_{j_1\leftrightarrow j_3}+T_{j_2\leftrightarrow j_3})$, and finally $j_1\neq j_2\neq j_3\neq j_1$, $\sigma(T)=\{1\}$ to $T^S=6^{-\frac{1}{2}}\sum_{\pi\in S_3}T_\pi$ (the subscript indicates the permutation performed on the edges and their labellings). These are all independent states which survive group averaging. We see that essentially we come back to the gauge-fixed states with only three fixed edges, the only novelty being implied by the symmetrization with respect to S_3 . But there are still the three

labels j_1 , j_2 and j_3 , and certainly the vertex contractor which are all needed to specify a state. The symmetrization implies only a minor decrease in the freedom. In contrast, if we treat SO(3) as a symmetry group for an isotropic model, we have seen that there remains only one edge labelled by a single spin j, and the insertion mentioned earlier, which can be viewed as a remnant of the vertex contractor. This illustrates the difference between the different treatments of symmetry and gauge: solving the gauge constraint eliminates redundant degrees of freedom which are given by the ability to choose an arbitrary dreibein to represent the edges (interpreted in terms of the auxiliary manifold). The symmetry reduction reduces the number of degrees of freedom even more by selecting particular geometries, and therefore the number of spin network labels is reduced.

The diffeomorphism constraint for isotropic models vanishes identically, which is consistent with the discussion above: symmetry reduction is stronger than gauge reduction, and therefore an isotropic state is automatically invariant with respect to inner automorphisms.

For LRS models the situation is different: here, the constraint (10) either vanishes identically $(n^{(1)} + n^{(2)} = 0)$ or is equivalent to the Gauß constraint, i.e. it is already solved by using gauge-invariant states. This is a consequence of the Higgs constraint, which can most easily be seen in the form (14). For LRS models we have $n^{(1)} = n^{(2)}$ (see [27]), which is non-zero in the case of a non-vanishing diffeomorphism constraint. In this case the only inner automorphism with respect to which there is a non-vanishing component of the diffeomorphism constraint is a rotation around the axial edge. But owing to the Higgs constraint (14) such a rotation applied to a transversal edge is equivalent to a gauge rotation of the associated holonomy. This observation explains the fact that the diffeomorphism constraint is equivalent to the Gauß constraint in those cases. For $n^{(1)} = 0$, on the other hand, there is no inner automorphism in the transversal plane and no diffeomorphism constraint is needed.

6. Conclusion

In this paper we have presented the basic setting for the study of cosmological models within loop quantum gravity. The kinematical level has been almost completely solved. It remains to determine the quantum states which solve the Higgs constraint. This will be done in the next part, together with a quantization of volume operators for cosmological models.

In this early stage, of course, no physical statements concerning features of a quantum theory of gravity in a cosmological context can be made. Instead we have concentrated on an application of these models as test models for the general framework of quantum symmetry reduction presented in [20]. Cosmological models are well suited for that task, because in the quantum formulation they consist of a Higgs vertex only. This allows us to study these vertices, the treatment of which has not yet been addressed in the general framework (for a non-trivial Higgs constraint). In the next part of this series (following paper) we will complete the solution of the Higgs constraint for isotropic models, and show how spin network techniques can be used on the solution space. Furthermore, the models discussed here again illustrate the role of the reduced gauge group and of the relaxing of a partial gauge fixing in the quantum theory.

Once we have the reduced models and their complete kinematical Hilbert spaces at our disposal, we can use them as test models for poorly understood issues of the full theory. The history of physics provides many examples of how important the role of models with high symmetry can be. For most theories the only known exact solutions are highly symmetric, and such solutions can provide insights into conceptual issues. Therefore, it should be helpful to use symmetric states to investigate problems of loop quantum gravity. The outstanding task is, of course, to understand the Hamiltonian constraint. The action of a candidate [18, 19] for its quantization is already complicated in a single vertex, and for its full action one has to take into

account the whole spin network it acts on by creating new edges. For cosmological models, there is just a single vertex. No new edges can be created; only the spins can be changed. Thus already the simple geometry implies a simplification (an example for such a simplification is the discussion of group averaging of the diffeomorphism group for Bianchi IX models presented in the preceding section). Moreover, the Wheeler–DeWitt operator contains the volume operator, whose eigenvalues are not known explicitly for complicated vertices. For isotropic models there are only specific vertices, and we will see in the next part that the complete spectrum of the volume operator can be calculated. This should further facilitate an investigation of the reduced Hamiltonian constraint. Lastly, we mention that the classical isotropic solutions are known explicitly and are very simple, so a comparison with the classical theory will be easier to achieve. A quantization of Wheeler–DeWitt operators for homogeneous models will be presented in the third part [21] of this series.

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