

Perturbative Degrees of Freedom in Loop Quantum Gravity: Anisotropies

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Abstract

The relation between an isotropic and an anisotropic model in loop quantum cosmology is discussed in detail, comparing the strict symmetry reduction with a perturbative implementation of symmetry. While the latter cannot be done in a canonical manner, it allows to consider the dynamics including the role of small non-symmetric degrees of freedom for the symmetric evolution. This serves as a model for the general situation of perturbative degrees of freedom in a background independent quantization such as loop quantum gravity, and for the more complicated addition of perturbative inhomogeneities. While being crucial for cosmological phenomenology, it is shown that perturbative non-symmetric degrees of freedom do not allow definitive conclusions for the singularity issue and in such a situation could even lead to wrong claims.

1 Introduction

By far the most common and extended studies in cosmological models are those admitting only finitely many or even one gravitational degree of freedom, the scale factor or radius of the universe $a(t)$ and maybe anisotropy parameters. This is justified in a homogeneous or isotropic model, symmetries present in our universe at large scales. This is also mainly implemented in models of quantum gravity, such as in Wheeler–DeWitt quantum cosmology [1, 2] and loop quantum cosmology [3, 4, 5]. That degree of symmetry does not only allow

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insights into phenomenological aspects of the early universe but, in anisotropic models, also displays the most crucial features of classical singularities.

More realistic models can then be obtained by breaking some of the symmetries imposed as before. After isotropy the first step is anisotropy, which can often be implemented exactly, and then inhomogeneity as the crucial one. In the first case (anisotropy) there is still a finite number of degrees of freedom and usually they do not pose much new technical difficulties. Conceptually, however, they are essential in particular for a general understanding of the issue of singularities (see, e.g., [6] for a recent discussion in the context of quantum cosmology). It is then of interest to discuss anisotropic models at different levels and to see what the implications for singularities are. Complete quantizations have been done in [7, 8, 9] with the result that their loop quantizations are free of singularities as in isotropic cases [10, 11, 12].

Alternatively, one can try to implement anisotropies as perturbations to a quantized isotropic model and see how correction terms change the dynamical behavior. In this work we develop such a point of view both to shed light on the singularity issue and as a model for perturbative inhomogeneities. Following [7] where anisotropic models have been quantized in the loop framework, we introduce suitable anisotropy parameters in that model and implement conditions for them to be small. (As a first step we take only one anisotropy parameter of two possible ones which means that there is still a single rotational symmetry axis, a so-called locally rotationally symmetric (LRS) situation.) This will be discussed in detail at the kinematical and dynamical levels and results in an evolution equation describing an anisotropic model perturbatively around an isotropic one. The formulation can also be used for comparing background independent theories with theories formulated on a background, because the isotropic model can be seen as a background for the perturbative anisotropy.

In section 2 we describe the classical models, to be quantized in section 3 both exactly and in a perturbative manner. This illustrates how symmetric models can be related to a less symmetric theory at the quantum level. In section 4 we discuss the evolution equation in terms of the perturbation and its new features compared to the isotropic model. In section 5 we look at the singularity issue from the perturbative point of view and show that conclusions drawn in such a situation must be used much more carefully than in a non-perturbative quantization.

2 Classical models

For simplicity, we consider the two most simple models, which are the flat isotropic model and the Bianchi I model with one additional rotational symmetry (LRS). Since loop quantizations are based on Ashtekar variables [13, 14] given by a connection A_a^i and a densitized triad E_i^a we first introduce these variables. In models, they take special forms corresponding to the fact that they are required to be preserved by a symmetry transformation up to a gauge transformation.

An isotropic connection and densitized triad for a flat model can always be written as

$$A_a^i dx^a = \bar{c} dx^i \quad (1)$$

$$E_i^a \frac{\partial}{\partial x^a} = \bar{p} \frac{\partial}{\partial x^i} . \quad (2)$$

in Cartesian coordinates, where the only two remaining components are conjugate to each other,

$$\{\bar{c}, \bar{p}\} = \frac{8\pi}{3} \gamma G \quad (3)$$

with the Barbero–Immirzi parameter γ [14, 15] and the gravitational constant G . The variable \bar{p} contains information about spatial geometry such as the volume

$$V_{\text{iso}} = |\bar{p}|^{3/2} \quad (4)$$

while \bar{c} is proportional to extrinsic curvature. Both variables are related dynamically as dictated by the Hamiltonian constraint

$$H_{\text{iso}} = -\frac{3}{8\pi G \gamma^2} \bar{c}^2 \sqrt{|\bar{p}|} + H_{\text{matter}}(\bar{p}) = 0 . \quad (5)$$

Similarly, in the LRS Bianchi I model we have

$$A_a^i dx^a \tau_i = A \tau^1 dx + A \tau^2 dy + c \tau^3 dz \quad (6)$$

$$E_i^a \frac{\partial}{\partial x^a} \tau^i = p_A \tau^1 \partial_x + p_A \tau^2 \partial_y + p_c \tau^3 \partial_z \quad (7)$$

with symplectic structure

$$\{A, p_A\} = 4\pi \gamma G , \quad \{c, p_c\} = 8\pi \gamma G . \quad (8)$$

There is a residual gauge transformation $p_A \mapsto -p_A$ which can be fixed by requiring $p_A \geq 0$ (see [7, 9] for more details). The volume is now given by

$$V_{\text{aniso}} = \sqrt{p_A^2 |p_c|} \quad (9)$$

and the Hamiltonian constraint by

$$H_{\text{aniso}} = -(8\pi G)^{-1} \gamma^{-2} (A^2 \sqrt{p_A} + 2Ac \sqrt{|p_c|}) + H_{\text{matter}}(p_A, p_c) = 0 . \quad (10)$$

To identify the anisotropy as a perturbation it is convenient to introduce new variables

$$(A, c) = (\bar{c} + \varepsilon, \bar{c} - 2\varepsilon) \quad (11)$$

$$(p_A, p_c) = (\bar{p} + p_\varepsilon, \bar{p} - 2p_\varepsilon) \quad (12)$$

together with the inverse transformation

$$(\bar{c}, \bar{p}) = \left(\frac{1}{3}(2A + c), \frac{1}{3}(2p_A + p_c) \right) \quad (13)$$

$$(\varepsilon, p_\varepsilon) = \left(\frac{1}{3}(A - c), \frac{1}{3}(p_A - p_c) \right) \quad (14)$$

as well as the symplectic structure

$$\{\bar{c}, \bar{p}\} = \frac{8\pi}{3}\gamma G, \quad \{\varepsilon, p_\varepsilon\} = \frac{4\pi}{3}\gamma G. \quad (15)$$

The volume, in this manner, is given by \bar{p} up to terms of at least second order in p_ε , which is the motivation for choosing our particular set of anisotropy variables:

$$V_{\text{aniso}} = \sqrt{|\bar{p}^3 - 3p_\varepsilon^2\bar{p} - 2p_\varepsilon^3|} = |\bar{p}|^{3/2} \left(1 - \frac{3p_\varepsilon^2}{2\bar{p}^2} + O(p_\varepsilon^3/\bar{p}^3) \right). \quad (16)$$

This shows that we have to assume $p_\varepsilon \ll \bar{p}$ for perturbations, i.e. the approximation will break down close to classical singularities of the isotropic type where $\bar{p} = 0$. Later, we will also have to assume $\varepsilon \ll 1$. For the Hamiltonian constraint we obtain

$$H_{\text{aniso}} = -\frac{3}{8\pi G\gamma^2} |\bar{p}|^{-3/2} (\bar{c}^2\bar{p}^2 - \varepsilon^2\bar{p}^2 - \bar{c}^2p_\varepsilon^2 + 2\bar{c}\bar{p}\varepsilon p_\varepsilon + O(p_\varepsilon^3/\bar{p}^3)) + H_{\text{matter}}(\bar{p}, p_\varepsilon) \quad (17)$$

up to terms of third order in the perturbation.

In the vacuum case, we have Hamiltonian equations of motion

$$\dot{\bar{c}} = \{\bar{c}, H_{\text{aniso}}\} \propto -\bar{c}^2\bar{p} + \varepsilon^2\bar{p} - \bar{c}\varepsilon p_\varepsilon \quad (18)$$

$$\dot{\bar{p}} = \{\bar{p}, H_{\text{aniso}}\} \propto \bar{c}\bar{p}^2 - \bar{c}p_\varepsilon^2 + \bar{p}\varepsilon p_\varepsilon \quad (19)$$

$$\dot{\varepsilon} = \{\varepsilon, H_{\text{aniso}}\} \propto \frac{1}{2}\bar{c}^2 p_\varepsilon - \frac{1}{2}\bar{c}\bar{p}\varepsilon \quad (20)$$

$$\dot{p}_\varepsilon = \{p_\varepsilon, H_{\text{aniso}}\} \propto -\frac{1}{2}\bar{p}^2\varepsilon + \frac{1}{2}\bar{c}\bar{p}p_\varepsilon. \quad (21)$$

Thus, the isotropic variables receive corrections in their equations of motion only at second order. Ignoring those corrections, we recover the classical solution $\bar{c} = 0$ and $\bar{p} = \text{const}$ for flat Minkowski space. With this approximate solution for the anisotropic system, the equations for anisotropies simplify to $\dot{\varepsilon} \approx 0$ and $\dot{p}_\varepsilon \approx -\frac{1}{2}\bar{p}^2\varepsilon$. The anisotropy in the connection will thus remain constant while that in the triad grows linearly in time until the approximations break down. Since the constraint is quadratic in connection components, a feature shared by the full constraint, we are not required at this point to assume $\varepsilon \ll 1$. However, the equations of motion show that \dot{p}_ε would be large if ε is not small, and we are led to this condition if the perturbative evolution is to be valid for some time.

We will later, at the quantum level, mainly consider an asymptotic approximation of very large \bar{p} where all corrections of higher order in p_ε/\bar{p} are ignored. This also simplifies the classical equations because the Hamiltonian constraint is then simply proportional to $-(\bar{c}^2 - \varepsilon^2)\sqrt{|\bar{p}|}$. Notice that the quadratic nature of the constraint in connection variables makes this approximation reasonable as we do not need to expand in ε . The solution $\varepsilon = \bar{c}$ to the constraint is thus consistent even though the anisotropy ε in the connection is not small compared to \bar{c} (unlike p_ε which must be small compared to \bar{p}). As already mentioned, and used later, it is only necessary that ε is small compared to one, which is usually the case also for \bar{c} in semiclassical regimes.

Using the large- \bar{p} constraint we have equations of motion

$$\begin{aligned}\dot{\bar{c}} &= -\frac{\bar{c}^2}{2\sqrt{|\bar{p}|}} + \frac{\varepsilon^2}{2\sqrt{|\bar{p}|}} \approx 0 \\ \dot{\bar{p}} &= 2\bar{c}\sqrt{|\bar{p}|} \\ \dot{\varepsilon} &= 0 \\ \dot{p}_\varepsilon &= -\varepsilon\sqrt{|\bar{p}|}.\end{aligned}$$

With $\varepsilon = \bar{c} = \text{const}$ we have $\bar{p} = (\varepsilon t + \sqrt{|\bar{p}_0|})^2$ and $p_\varepsilon = p_\varepsilon^0 - \frac{1}{2}\varepsilon^2 t^2 - \varepsilon\sqrt{|\bar{p}_0|}t$ with constants of integration \bar{p}_0 and p_ε^0 . Eliminating t , we have the internal time evolution

$$p_\varepsilon(\bar{p}) = p_\varepsilon^0 - \frac{1}{2}(\bar{p} - \bar{p}_0) \quad (22)$$

of p_ε with respect to \bar{p} . Notice that this evolution, unlike the coordinate time evolution, does not depend on the value of ε . We will use this fact later as a test of the perturbative quantum evolution.

3 Quantization

Loop quantizations are based on holonomies, and also in models one uses exponentials of connection components as basic expressions in addition to densitized triad components. In the isotropic case, this leads to a basic algebra given by p and $\exp(i\mu\bar{c}/2)$ for all $\mu \in \mathbb{R}$, represented on a non-separable Hilbert space

$$\mathcal{H}_{\text{iso}} \cong L^2(\mathbb{R}_{\text{Bohr}}, d\mu_{\text{H}}) \quad (23)$$

of square integrable functions on the Bohr compactification of the real line [12], with orthonormal basis

$$\langle \bar{c}|\mu\rangle = \exp(i\mu\bar{c}/2) \quad , \quad \mu \in \mathbb{R} \quad (24)$$

and basic operators acting as

$$\widehat{\exp(i\mu'\bar{c}/2)}|\mu\rangle = |\mu + \mu'\rangle \quad (25)$$

$$\hat{p}|\mu\rangle = \frac{1}{6}\gamma\ell_{\text{P}}^2\mu|\mu\rangle \quad (26)$$

using the Planck length $\ell_{\text{P}} = \sqrt{8\pi G\hbar}$. Similarly, for our anisotropic model we have the Hilbert space

$$\mathcal{H}_{\text{aniso}} \cong \mathcal{H}_{\text{iso}} \otimes \mathcal{H}_{\text{iso}} \quad (27)$$

with orthonormal basis

$$\langle A, c|\mu, \nu\rangle = \exp(i(\mu c + \nu A)/2) \quad , \quad \mu, \nu \in \mathbb{R} \quad (28)$$

holonomy operators as before and

$$\hat{p}_A|\mu, \nu\rangle = \frac{1}{4}\gamma\ell_{\text{P}}^2\mu|\mu, \nu\rangle \quad , \quad \hat{p}_c|\mu, \nu\rangle = \frac{1}{2}\gamma\ell_{\text{P}}^2\nu|\mu, \nu\rangle. \quad (29)$$

These states are not completely gauge invariant in view of the residual gauge transformation $\mu \mapsto -\mu$, which however will not be relevant for our purposes. One can always ensure gauge invariance by working only with states $\sum_{\mu,\nu} \psi_{\mu,\nu} |\mu, \nu\rangle$ where $\psi_{\mu,\nu}$ is symmetric in μ . The triad operators then give us directly the volume operators for both models by inserting them into the classical expressions.

For mathematical constructions one often makes use of dense subspaces Cyl_{iso} and $\text{Cyl}_{\text{aniso}}$ of the two Hilbert spaces given by the so-called cylindrical functions which are finite linear combinations of the basis states $|\mu\rangle$ or $|\mu, \nu\rangle$, respectively. With their algebraic duals of distributional states (linear functionals on the cylindrical subspaces) one has two Gel'fand triples $\text{Cyl}_{\text{iso}} \subset \mathcal{H}_{\text{iso}} \subset \text{Cyl}_{\text{iso}}^*$ and $\text{Cyl}_{\text{aniso}} \subset \mathcal{H}_{\text{aniso}} \subset \text{Cyl}_{\text{aniso}}^*$ (see also [16]).

3.1 Symmetry reduction

Since we are interested in the relation between a symmetric model and a less symmetric one we first use the opportunity to demonstrate how a reduced model can be obtained within quantum theory (see also [17, 18, 5]). We start with the anisotropic model and, following general constructions [17], define an isotropic state as a distribution which is supported only on isotropic connections, i.e. $\varepsilon = 0$. To fulfill the definition, we must find an antilinear map

$$\sigma: \text{Cyl}_{\text{iso}} \rightarrow \text{Cyl}_{\text{aniso}}^*, |\mu\rangle \mapsto \langle \mu | \quad (30)$$

embedding the space of isotropic cylindrical functions into the distributional dual of the anisotropic one such that

$$\sigma(|\mu\rangle)[|\rho, \tau\rangle] = \langle \mu | \rho, \tau \rangle|_{A=c} \quad \text{for all } |\rho, \tau\rangle.$$

On the right hand side, we use the restriction of a state $|\rho, \tau\rangle$ to the subspace $A = c$ upon which it can be interpreted as an isotropic state. Expanding $\sigma(|\mu\rangle) =: \sum_{\kappa,\lambda} \sigma_{\kappa,\lambda}(\mu) \langle \kappa, \lambda |$, we have

$$\sigma_{\rho,\tau}(\mu) = \sum_{\kappa,\lambda} \sigma_{\kappa,\lambda}(\mu) \delta_{\kappa,\rho} \delta_{\lambda,\tau} = \sigma(|\mu\rangle)[|\rho, \tau\rangle] = \int e^{-i\mu c/2} e^{i(\rho+\tau)c/2} d\mu_{\text{H}}(c) = \delta_{\mu,\rho+\tau}$$

and thus

$$\langle \mu | = \sigma(|\mu\rangle) = \sum_{\kappa,\lambda} \delta_{\mu,\kappa+\lambda} \langle \kappa, \lambda | = \sum_{\kappa} \langle \kappa, \mu - \kappa |. \quad (31)$$

The summation is done over all real numbers, which is well-defined as a distribution in $\text{Cyl}_{\text{aniso}}^*$.

In fact, in this case the definition simply amounts to multiplying an isotropic state in the connection representation with a δ -distribution supported at $\varepsilon = 0$,

$$\sigma(|\mu\rangle)|A, c\rangle = \sum_{\kappa} e^{i(\kappa A + (\mu - \kappa)c)/2} = e^{i\mu c/2} \sum_{\kappa} e^{i\kappa(A-c)/2} = e^{i\mu c/2} \delta(A - c)$$

but this would be more complicated in more general systems and the full theory where the definitions of [17] still apply.

Indeed, this gives $\langle \mu | \rho, \tau \rangle = \delta_{\mu, \rho + \tau}$, i.e. the evaluation of the distribution is non-zero only if the averaged label equals the isotropic one,

$$\frac{1}{2}\gamma\ell_{\mathbb{P}}^2(\rho + \tau) = 2(\hat{p}_A)_\rho + (\hat{p}_c)_\tau = 3(\hat{\bar{p}})_{\rho + \tau}$$

and $\langle \mu | h_A^{(\rho)} h_c^{(\rho)-1} = \langle \mu |$, i.e. $\exp(i\rho\varepsilon)$ acts trivially with its dual action on symmetric distributions which are thus supported only on isotropic connections $\varepsilon = 0$.

Here, we already used the dual action of anisotropic operators on isotropic distributional states, which in this example mapped a symmetric state to a symmetric one. This is not the case for arbitrary operators, and one cannot simply define all operators for the reduced model by the dual action of anisotropic operators [18]. However, one can do this for special operators which suffice to define the basic operators of the model. For flux operators, one can easily see that $2\hat{p}_A + \hat{p}_c = 3\hat{\bar{p}}$ is the only one which maps an isotropic state $\langle \mu |$ to an isotropic state:

$$\hat{p}\sigma(|\mu\rangle) = \frac{1}{3}\langle \mu | (2\hat{p}_A + \hat{p}_c) = \frac{1}{6}\gamma\ell_{\mathbb{P}}^2\mu(|\mu\rangle = \sigma(\hat{\bar{p}}|\mu\rangle). \quad (32)$$

Moreover, it agrees with the isotropic flux operator (26) defined in the isotropic model. For holonomies, one can act with arbitrary products of h_A and h_c on isotropic states since we already know that $h_A h_c^{-1}$ acts as the identity and the remaining factor simply amounts to an isotropic holonomy operator. Also, all holonomy operators form a closed algebra with the isotropic flux operator $\hat{\bar{p}} = \frac{1}{3}(2\hat{p}_A + \hat{p}_c)$:

$$[h_A^{(\rho)} h_c^{(\tau)}, \hat{\bar{p}}]|\mu, \nu\rangle = -\frac{1}{6}\gamma\ell_{\mathbb{P}}^2(\rho + \tau)|\mu + \rho, \nu + \tau\rangle = -\frac{1}{6}\gamma\ell_{\mathbb{P}}^2(\rho + \tau)h_A^{(\rho)} h_c^{(\tau)}|\mu, \nu\rangle. \quad (33)$$

This is similar for the anisotropy operator which we can define by $\hat{p}_\varepsilon := \frac{1}{3}(\hat{p}_A - \hat{p}_c)$. Here, we have the commutator

$$[h_A^{(\rho)} h_c^{(\tau)}, \hat{p}_\varepsilon] = -\frac{1}{6}\gamma\ell_{\mathbb{P}}^2(\frac{1}{2}\rho - \tau)h_A^{(\rho)} h_c^{(\tau)}. \quad (34)$$

However, \hat{p}_ε does not map an isotropic distribution to another such distribution.

If we are looking for a reduction of the operator algebra to implement isotropy, we need to find distinguished dual actions making use of the form of symmetric states. One clearly distinguished operator is $\hat{\bar{p}}$ because it is the only flux operator mapping an isotropic distributional state to another such state. For holonomies, $h_A h_c^{-1}$ is distinguished because it fixes any isotropic distributional state. Beyond that, no other operators are intrinsically distinguished, but we do not yet have a useful algebra of operators for an isotropic model: while \bar{p} is available, our distinguished holonomy corresponds to the anisotropy ε rather than the conjugate of \bar{p} . Nevertheless, by acting with the distinguished $\hat{\bar{p}}$ as well as *all* holonomy operators, we can generate the isotropic representation. More precisely, we define

$$\text{Stab}(\sigma) := \{\hat{O} \in \mathcal{A}_{\text{aniso}} | \hat{O}\sigma(\text{Cyl}_{\text{iso}}) \subset \sigma(\text{Cyl}_{\text{iso}})\} \quad (35)$$

and

$$\text{Fix}(\sigma) := \{\hat{O} \in \mathcal{A}_{\text{aniso}} | \hat{O}\sigma(\psi) = \sigma(\psi) \text{ for all } \psi \in \text{Cyl}_{\text{iso}}\}. \quad (36)$$

The isotropic algebra is then

$$\mathcal{A}_{\text{iso}} := \text{Stab}(\sigma)/\text{Fix}(\sigma) \quad (37)$$

understood in the following manner: $\text{Fix}(\sigma)$ contains only holonomy operators besides the identity, and thus forms a normal subgroup of the Abelian group obtained from the multiplicative operation in the holonomy algebra. We can thus take the factor group of holonomy operators modulo $\text{Fix}(\sigma)$ which thanks to the distributive law can also be equipped with the usual additive structure to form an algebra. Due to the relation (33), also the flux operators in $\text{Stab}(\sigma)$ commute with $\text{Fix}(\sigma)$ and thus descend to the factor group, defining \mathcal{A}_{iso} . Using that $\text{Stab}(\sigma)$ is generated as an algebra by \hat{p} and all $h_A^{(\rho)} h_c^{(\tau)}$ and $\text{Fix}(\sigma)$ by $h_A h_c^{-1}$, a general element of \mathcal{A}_{iso} is

$$\left(\sum_{n \in \mathbb{N}_0} \hat{p}^n \pi_n(h_c) \right) \cdot \text{Fix}(\sigma)$$

with Laurent polynomials π_n , allowing also inverse powers of h_c , for each n which are non-zero only for finitely many n (we can order \hat{p} to the left using (33) and factor out a power of $h_A h_c^{-1}$ into $\text{Fix}(\sigma)$ such that only the holonomy h_c appears explicitly). Through this construction we derive an algebra isomorphic to the isotropic one.

As the presence of factor spaces indicates, there is no canonical isotropic subalgebra of the anisotropic algebra without additional input. This is analogous to the classical situation where the splitting of anisotropic variables A and c into an isotropic average \bar{c} and an anisotropy is not unique. Classically, a given \bar{p} , as we have it distinguished at the quantum level, determines a form of ε as a linear combination of A and c by requiring $\{\bar{p}, \varepsilon\} = 0$. Indeed, also the quantum analog of ε , given by $h_A h_c^{-1}$, is distinguished as it commutes with \hat{p} . However, a unique form for \bar{c} and p_ε then follows only after an additional choice, which for us was the fact that the volume should receive corrections only to second order. We use this here to define $\hat{p}_\varepsilon = \frac{1}{3}(\hat{p}_A - \hat{p}_c)$ as above and then require that (34) vanish, analogously to $\{\bar{c}, p_\varepsilon\} = 0$. This distinguishes $h_A^2 h_c$ as the isotropic holonomy operator in addition to the flux \hat{p} which indeed form a subalgebra of the anisotropic operator algebra mapping isotropic states to isotropic states in a way isomorphic to the isotropic model.

In this manner, we obtain a unique subalgebra of the basic anisotropic operator algebra which is isomorphic to the basic isotropic algebra. This also presents an alternative way to define a symmetric model without referring to symmetric distributional states at all: we use the classical relations between symmetric and non-symmetric variables to define a distinguished algebra derived from the non-symmetric holonomy-flux algebra. Using the fact that the non-symmetric representation is cyclic on $|0, 0\rangle$, i.e. the subspace $\mathcal{A}_{\text{aniso}}|0, 0\rangle$ is dense in $\mathcal{H}_{\text{aniso}}$, we generate the representation of the reduced model by acting only with the subalgebra on the cyclic state. This defines the reduced state space, which is equipped with an inner product by requiring holonomy operators to be unitary. Upon completion, this inner product space defines the Hilbert space of the isotropic model and its quantum representation in agreement with the loop quantization of the classically reduced model.

Characteristic properties of the representation are then clearly inherited from that of the less symmetric system, which in some cases is also visible for the reduction from the full theory [18, 5].

3.2 Perturbations

Dynamical information is obtained by quantizing the Hamiltonian constraints and asking physical states to be annihilated by the resulting operators. Because the constraints contain connection components, and connections are represented via holonomies which shift the labels of states as in (25), quantum constraint equations become difference equations [19, 10, 7] for states $|\psi\rangle = \sum_{\mu} \psi_{\mu} |\mu\rangle$ or $|\psi\rangle = \sum_{\mu, \nu} \psi_{\mu, \nu} |\mu, \nu\rangle$ in the triad representation. For large scales, e.g. $\mu \gg 1$ in the isotropic case, the difference equation is well-approximated by the Wheeler–DeWitt equation [20] while for small μ there are crucial differences implying the absence of singularities at the quantum level [11]. In order to see the relation to the Wheeler–DeWitt equation, one has to assume that the wave function does not vary rapidly on small scales, i.e. changes in μ of the order one, which allows one to Taylor expand the difference operators into differential ones. This limit, however, does not exist for arbitrary states because there is no operator for \bar{c} on \mathcal{H}_{iso} [12]. Indeed, the Wheeler–DeWitt quantization is based on a representation on the usual Schrödinger Hilbert space $\mathcal{H}_{\text{S}} = L^2(\mathbb{R}, d\bar{c})$ which is inequivalent to the representation on the Bohr Hilbert space used for the loop quantization.

In this paper, we analyze the case of an anisotropic model where, however, difference operators are not expanded for both triad components but only for that corresponding to the anisotropy p_{ε} . We thus assume that the wave function does not vary rapidly when p_{ε} changes and that in an approximate sense an operator for ε exists. Although we need to assume p_{ε} to be small, this will not push us in the regime where discreteness is relevant provided that \bar{p} is large. The key additional assumption is that ε is not too big which now becomes important at the quantum level, and indeed both anisotropy parameters, p_{ε} and ε , have to be small. (The situation is different from pure isotropy where small \bar{p} usually implies large \bar{c} .) When only small ε are allowed, we do not probe the whole configuration space and do not see its compactness which underlies the Bohr Hilbert space used in homogeneous loop quantizations. As in the large volume limit, we therefore introduce the Schrödinger Hilbert space \mathcal{H}_{S} for anisotropies, which we do by defining the perturbative Hilbert space

$$\mathcal{H}_{\text{pert}} := \mathcal{H}_{\text{iso}} \otimes \mathcal{H}_{\text{S}} \tag{38}$$

and realizing its dense subset $\text{Cyl}_{\text{iso}} \otimes \text{Cyl}_{\text{S}}$ as a subspace of the dual $\text{Cyl}_{\text{aniso}}^*$. In the Schrödinger Hilbert space we have to choose a suitable dense set Cyl_{S} , which for our purposes will be the set of all functions which are products of a polynomial and a Gaussian. Indeed, Schrödinger states in Cyl_{S} can be interpreted as distributions on the Bohr Hilbert space [21] using the antilinear map

$$\pi: \text{Cyl}_{\text{S}} \rightarrow \text{Cyl}_{\text{Bohr}}^*, \pi(\psi)[|\rho\rangle] := \int e^{i\rho\varepsilon} \overline{\psi(\varepsilon)} d\varepsilon.$$

Dual actions of basic operators on those states are given by

$$\begin{aligned} (\hat{p}_\varepsilon \pi(\psi)) [|\rho\rangle] &= \pi(\psi) [\hat{p}_\varepsilon^\dagger |\rho\rangle] = \frac{1}{6} \gamma \ell_P^2 \int \rho e^{i\rho\varepsilon} \overline{\psi(\varepsilon)} d\varepsilon = \frac{1}{6} \gamma \ell_P^2 \int e^{i\rho\varepsilon} \cdot i \frac{d}{d\varepsilon} \overline{\psi(\varepsilon)} d\varepsilon \quad (39) \\ &= \pi(-\frac{1}{6} i \gamma \ell_P^2 d\psi/d\varepsilon) [|\rho\rangle] \end{aligned}$$

and

$$(e^{i\tau\varepsilon} \pi(\psi)) [|\rho\rangle] = \psi[e^{-i\tau\varepsilon} |\rho\rangle] = \int e^{i(\rho-\tau)\varepsilon} \overline{\psi(\varepsilon)} d\varepsilon = \int e^{i\rho\varepsilon} \overline{e^{i\tau\varepsilon} \psi(\varepsilon)} d\varepsilon = \pi(e^{i\tau\varepsilon} \psi) [|\rho\rangle]. \quad (40)$$

The first equation shows that the momentum operator is just the derivative operator, as also on the Bohr Hilbert space, while the second shows that $(e^{i\tau\varepsilon} \pi(\psi))(\varepsilon) = e^{i\tau\varepsilon} \psi(\varepsilon)$ where on the Schrödinger Hilbert space we can now take the derivative with respect to ν . By going to the dual action on the image of π , we thus obtain a simple multiplication operator for ε well-defined with domain $\pi(\text{Cyl}_S)$.

In addition, if we choose an appropriate state $\Psi \in \text{Cyl}_S$ we have an embedding $\text{id} \otimes \Psi: \text{Cyl}_{\text{iso}} \rightarrow \text{Cyl}_{\text{pert}}$ of isotropic cylindrical states to perturbative cylindrical states where anisotropies are small in mean value, but not eliminated exactly. Moreover, since we have to choose a state Ψ , which in the above notation is identified with the map $\mathbb{C} \rightarrow \text{Cyl}_S, 1 \mapsto \Psi$, there is no unique canonical embedding. (Coherent states are natural candidates, but unlikely to be preserved dynamically.) In addition to the strict implementation of symmetries σ we then have the perturbative implementation $\pi_\Psi := (\star \otimes \pi) \circ (\text{id} \otimes \Psi)$ which are both maps from Cyl_{iso} to $\text{Cyl}_{\text{aniso}}^*$:

$$\begin{array}{ccc} \begin{array}{c} \text{Cyl}_{\text{iso}}^* \\ \cup \\ \mathcal{H}_{\text{iso}} \\ \cup \\ \text{Cyl}_{\text{iso}} \end{array} & \begin{array}{c} \xrightarrow{\sigma} \\ \xrightarrow{\star \otimes \pi} \end{array} & \begin{array}{c} \text{Cyl}_{\text{aniso}}^* \\ \cup \\ \mathcal{H}_{\text{aniso}} \\ \cup \\ \text{Cyl}_{\text{aniso}} \end{array} \\ & \xrightarrow{\text{id} \otimes \Psi} \text{Cyl}_{\text{iso}} \otimes \text{Cyl}_S = \text{Cyl}_{\text{pert}} & \end{array}$$

We have the two Gel'fand triples of the exact models on the left and right, with the canonical embedding σ of the reduced model through distributions implementing symmetries precisely. In between, we have the perturbative cylindrical space which is connected to the anisotropic side through the antilinear map π from Cyl_S , combined with the antilinear dualization \star of isotropic states.

In the perturbative sector, non-symmetric degrees of freedom are present but can be arranged to be unexcited at least for initial states of the evolution. In this sense, the situation is similar to the field theory example studied in [22] where non-symmetric field modes are included in their vacuum or other coherent states. In this case, the field theory vacuum is a natural candidate for the analog of Ψ . Perturbative states can then be thought of as states where only the symmetric modes have been excited but non-symmetric ones have been left in their vacua. This is technically similar to our construction of strictly symmetric states at the end of the preceding subsection where we used only symmetric

operators in order to generate all states of the symmetric model out of the non-symmetric cyclic state $|0, 0\rangle$. Indeed, for background independent systems in loop quantum gravity the analog of a ground state is the cyclic state where no geometry at all is excited. Thus, although physically the construction in [22] is closer to the perturbative situation here, technically it is analogous to the situation of the strict model. This illustrates crucial differences in the context of symmetries between quantum field theory on a background and a background independent quantization of gravity.

We have already discussed the relation between anisotropic operators and isotropic ones for the exact implementation of symmetry. For the perturbative implementation, the same relation exists for operators which do not depend on anisotropies, but we can now also act with other operators as we already saw for $\hat{\varepsilon}$ and \hat{p}_ε in (40) and (39). In general, an anisotropic operator \hat{O} acting on $\mathcal{H}_{\text{aniso}}$ has a dual action on $\star \otimes \pi(\text{Cyl}_{\text{pert}}^*)$, but does not necessarily fix this subspace of $\text{Cyl}_{\text{aniso}}^*$. However, it does so perturbatively when we expand it as a sum of operators in the perturbative sector. Choosing, for definiteness, a Gaussian for Ψ we have perturbative states of the form

$$\psi(A, c) = e^{i\bar{\nu}c/2} e^{-(\varepsilon-\varepsilon_0)^2/4\sigma^2} e^{6i\varepsilon p_\varepsilon^0/\gamma\ell_P^2}$$

where $\bar{c} = \frac{1}{3}(2A + c)$ and $\varepsilon = \frac{1}{3}(A - c)$ are understood as functions of A and c . By the chain rule, we then have flux operators

$$\hat{p}_A \psi = -\frac{i}{2} \gamma \ell_P^2 \frac{\partial}{\partial A} \psi = -\frac{i}{6} \gamma \ell_P^2 \left(2 \frac{\partial}{\partial \bar{c}} + \frac{\partial}{\partial \varepsilon} \right) \psi = \left(\frac{1}{6} \gamma \ell_P^2 \bar{\nu} + \hat{p}_\varepsilon \right) \psi$$

and

$$\hat{p}_c \psi = -i \gamma \ell_P^2 \frac{\partial}{\partial c} \psi = -\frac{i}{3} \gamma \ell_P^2 \left(\frac{\partial}{\partial \bar{c}} - \frac{\partial}{\partial \varepsilon} \right) \psi = \left(\frac{1}{6} \gamma \ell_P^2 \bar{\nu} - 2\hat{p}_\varepsilon \right) \psi.$$

In composite expressions such as the volume operator one can then expand functions of flux operators in p_ε when they are expressed in the flux representation, and analogously for holonomy operators in the connection representation.

This is most easily done if eigenvalues are already known. For instance, if an operator \hat{O} has eigenstates $|\mu, \nu\rangle$, we take the eigenvalues $O_{\mu, \nu}$ and insert

$$\begin{aligned} \mu &= \frac{2}{3} \bar{\nu} + 4\gamma^{-1} \ell_P^{-2} p_\varepsilon = \frac{2}{3} \bar{\nu} + P, \\ \nu &= \frac{1}{3} \bar{\nu} - 4\gamma^{-1} \ell_P^{-2} p_\varepsilon = \frac{1}{3} \bar{\nu} - P \end{aligned} \quad (41)$$

with dimensionless $P := 4p_\varepsilon/\gamma\ell_P^2$, which follows from the classical relation (12) or the calculation above. This yields a function $O(\bar{\nu}, P)$ which we expand in the perturbation P ,

$$O(\bar{\nu}, P) = \sum_k O_{\text{iso}}^{(k)}(\bar{\nu}) P^k. \quad (42)$$

Note that P itself need not be small by our assumptions, which would mean $p_\varepsilon \ll \ell_P^2$. We have, however, $P \ll \bar{\nu}$ such that each $O_{\text{iso}}^{(k)}(\bar{\nu})$ must drop off at least as $\bar{\nu}^{-k}$. For

any fixed k , the values $O_{\text{iso}}^{(k)}(\bar{\nu})$, interpreted as eigenvalues, define an isotropic operator $\hat{O}_{\text{iso}}^{(k)} = \sum_{\bar{\nu}} O_{\text{iso}}^{(k)}(\bar{\nu}) |\bar{\nu}\rangle \langle \bar{\nu}|$ such that $\hat{O}_{\text{iso}}^{(k)} |\bar{\nu}\rangle := O_{\text{iso}}^{(k)}(\bar{\nu}) |\bar{\nu}\rangle$. Thus, we obtain the expansion

$$\hat{O} \sim \sum_k \hat{O}_{\text{iso}}^{(k)} \otimes \hat{P}^k \quad (43)$$

where the right hand side acts on $\mathcal{H}_{\text{pert}}$. This approximation of operators on a selected class of states implementing small anisotropy is discussed in more detail in App. A, which can be applied to any Hilbert space $|\bar{\nu}\rangle \otimes \mathcal{H}_{\text{S}}$ for fixed $\bar{\nu}$. We understand here always a finite truncation to a given order in k , and do not discuss convergence of the expansion in whatever sense. We will later use states Ψ of the above form, assuming $\sigma < \varepsilon_0 \ll 1$ in order to expand also in ε . This results in similar expansions for operators containing holonomies, such as the Hamiltonian constraint.

3.3 Hamiltonian constraint

The Hamiltonian constraint operator for the anisotropic model results from the expression given in [7] after using $A = c_1 = c_2$ and $c = c_3$ (as in [7], we ignore an ambiguity parameter μ_0 [12] which is of the order one and multiplies connection components in the constraint):

$$\begin{aligned} \hat{H} &= 4\pi^{-1} i \gamma^{-3} G^{-1} \ell_{\text{P}}^{-2} \left\{ \sin^2 \left(\frac{1}{2} A \right) \cos^2 \left(\frac{1}{2} A \right) \hat{O}_c + 2 \sin \left(\frac{1}{2} c \right) \cos \left(\frac{1}{2} c \right) \sin \left(\frac{1}{2} A \right) \cos \left(\frac{1}{2} A \right) \hat{O}_A \right\} \\ \hat{O}_c &:= \sin \left(\frac{1}{2} c \right) \hat{V} \cos \left(\frac{1}{2} c \right) - \cos \left(\frac{1}{2} c \right) \hat{V} \sin \left(\frac{1}{2} c \right) \end{aligned} \quad (44)$$

and similarly \hat{O}_A by replacing c by A , where \hat{V} is the anisotropic volume. Making use of the change of variables (13) one gets

$$\begin{aligned} \hat{H} &= 4\pi^{-1} i \gamma^{-3} G^{-1} \ell_{\text{P}}^{-2} \left\{ \sin^2 \left(\frac{1}{2} \bar{c} + \frac{1}{2} \varepsilon \right) \cos^2 \left(\frac{1}{2} \bar{c} + \frac{1}{2} \varepsilon \right) \hat{O}_c \right. \\ &\quad \left. + 2 \sin \left(\frac{1}{2} \bar{c} - \varepsilon \right) \cos \left(\frac{1}{2} \bar{c} - \varepsilon \right) \sin \left(\frac{1}{2} \bar{c} + \frac{1}{2} \varepsilon \right) \cos \left(\frac{1}{2} \bar{c} + \frac{1}{2} \varepsilon \right) \hat{O}_A \right\} \end{aligned} \quad (45)$$

Here \hat{O}_c and \hat{O}_A are more conveniently dealt with by using their action on the $|\mu, \nu\rangle$ basis, namely,

$$\hat{O}_A |\mu, \nu\rangle = \frac{i}{2} (V_{\mu+1, \nu} - V_{\mu-1, \nu}) |\mu, \nu\rangle \quad (46)$$

$$\hat{O}_c |\mu, \nu\rangle = \frac{i}{2} (V_{\mu, \nu+1} - V_{\mu, \nu-1}) |\mu, \nu\rangle \quad (47)$$

Now following (43) we expand \hat{O}_A and \hat{O}_c up to second order in p_ε , using from the exact analysis [7] that

$$V_{\mu, \nu} = \frac{1}{2} \left(\frac{1}{2} \gamma \ell_{\text{P}}^2 \right)^{\frac{3}{2}} \sqrt{\mu^2 |\nu|} = \frac{1}{2} \left(\frac{1}{2} \gamma \ell_{\text{P}}^2 \right)^{\frac{3}{2}} |\mu| \sqrt{|\nu|}. \quad (48)$$

Inserting (41), we obtain the eigenvalues

$$\begin{aligned} (O_A)_{\mu(\bar{\nu},P),\nu(\bar{\nu},P)} &= \frac{1}{4}i \left(\frac{1}{2}\gamma\ell_P^2\right)^{3/2} \left(|\frac{2}{3}\bar{\nu} + 1 + P| - |\frac{2}{3}\bar{\nu} - 1 + P|\right) \sqrt{|\frac{1}{3}\bar{\nu} - P|} \\ (O_c)_{\mu(\bar{\nu},P),\nu(\bar{\nu},P)} &= \frac{1}{4}i \left(\frac{1}{2}\gamma\ell_P^2\right)^{3/2} |\frac{2}{3}\bar{\nu} + P| \left(\sqrt{|\frac{1}{3}\bar{\nu} + 1 - P|} - \sqrt{|\frac{1}{3}\bar{\nu} - 1 - P|} \right). \end{aligned}$$

For $P \ll \bar{\nu}$, the absolute values can be evaluated as

$$\begin{aligned} |\frac{2}{3}\bar{\nu} + 1 + P| - |\frac{2}{3}\bar{\nu} - 1 + P| &= |\frac{2}{3}\bar{\nu} + 1| \left(1 + (\frac{2}{3}\bar{\nu} + 1)^{-1}P\right) - |\frac{2}{3}\bar{\nu} - 1| \left(1 + (\frac{2}{3}\bar{\nu} - 1)^{-1}P\right) \\ &= |\frac{2}{3}\bar{\nu} + 1| - |\frac{2}{3}\bar{\nu} - 1| + \left(\text{sgn}(\frac{2}{3}\bar{\nu} + 1) - \text{sgn}(\frac{2}{3}\bar{\nu} - 1)\right) P \\ &= 2\text{sgn}_{3/2}(\bar{\nu}) - 3\chi_{3/2}(\bar{\nu})P, \end{aligned}$$

introducing

$$\chi_\delta(\bar{\nu}) := -\frac{1}{2\delta}(\text{sgn}(\bar{\nu} + \delta) - \text{sgn}(\bar{\nu} - \delta)) = \begin{cases} 0 & \text{for } |\bar{\nu}| \geq \delta \\ \delta^{-1} & \text{for } |\bar{\nu}| < \delta \end{cases} \quad (49)$$

$$\text{sgn}_\delta(\bar{\nu}) := \frac{1}{2\delta}(|\bar{\nu} + \delta| - |\bar{\nu} - \delta|) = \begin{cases} 1 & \text{for } \bar{\nu} \geq \delta \\ \delta^{-1}\bar{\nu} & \text{for } |\bar{\nu}| < \delta \\ -1 & \text{for } \bar{\nu} \leq -\delta \end{cases}, \quad (50)$$

and

$$|\frac{2}{3}\bar{\nu} + P| = |\frac{2}{3}\bar{\nu}|(1 + 3P/2\bar{\nu})$$

while the other expressions are expanded as

$$\sqrt{|\frac{1}{3}\bar{\nu} - P|} = \sqrt{\frac{1}{3}\bar{\nu}} \left(1 - \frac{3}{2}P/\bar{\nu} - \frac{9}{8}P^2/\bar{\nu}^2 + O(P^3/\bar{\nu}^3)\right)$$

and

$$\begin{aligned} |\frac{1}{3}\bar{\nu} + 1 - P|^{1/2} - |\frac{1}{3}\bar{\nu} - 1 - P|^{1/2} &= |\frac{1}{3}\bar{\nu} + 1|^{1/2} \sqrt{1 - (\frac{1}{3}\bar{\nu} + 1)^{-1}P} \\ &\quad - |\frac{1}{3}\bar{\nu} - 1|^{1/2} \sqrt{1 - (\frac{1}{3}\bar{\nu} - 1)^{-1}P} \\ &= |\frac{1}{3}\bar{\nu} + 1|^{1/2} \left(1 - \frac{1}{2}(\frac{1}{3}\bar{\nu} + 1)^{-1}P - \frac{1}{8}(\frac{1}{3}\bar{\nu} + 1)^{-2}P^2\right) \\ &\quad - |\frac{1}{3}\bar{\nu} - 1|^{1/2} \left(1 - \frac{1}{2}(\frac{1}{3}\bar{\nu} - 1)^{-1}P - \frac{1}{8}(\frac{1}{3}\bar{\nu} - 1)^{-2}P^2\right) \\ &\quad + O(P^3/\bar{\nu}^3) \\ &= |\frac{1}{3}\bar{\nu} + 1|^{1/2} - |\frac{1}{3}\bar{\nu} - 1|^{1/2} \\ &\quad - \frac{1}{2} \left(|\frac{1}{3}\bar{\nu} + 1|^{-1/2} \text{sgn}(\frac{1}{3}\bar{\nu} + 1) - |\frac{1}{3}\bar{\nu} - 1|^{-1/2} \text{sgn}(\frac{1}{3}\bar{\nu} - 1) \right) P \\ &\quad - \frac{1}{8} \left(|\frac{1}{3}\bar{\nu} + 1|^{-3/2} - |\frac{1}{3}\bar{\nu} - 1|^{-1/2} \right) P^2 + O(P^3/\bar{\nu}^3) \\ &= 2\sqrt{3}\Delta_3\sqrt{|\bar{\nu}|} - 3\sqrt{3}P\Delta_3 \frac{\text{sgn}(\bar{\nu})}{\sqrt{|\bar{\nu}|}} \\ &\quad - \frac{9}{4}\sqrt{3}P^2\Delta_3|\bar{\nu}|^{-3/2} + O(P^3/\bar{\nu}^3) \end{aligned}$$

introducing, more generally than before,

$$\Delta_\delta f(\bar{\nu}) := \frac{1}{2\delta}(f(\bar{\nu} + \delta) - f(\bar{\nu} - \delta)) \quad (51)$$

for any function f which for functions differentiable at large $\bar{\nu}$ gives $\Delta_\delta f(\bar{\nu}) \sim f'(\bar{\nu})$ for $\bar{\nu} \gg \delta$.

This results in

$$\begin{aligned} \hat{O}_A &= \frac{1}{4\sqrt{3}}i \left(\frac{1}{2}\gamma\ell_P^2\right)^{3/2} \sqrt{|\hat{\nu}|} \left(2\text{sgn}_{3/2}(\hat{\nu}) \otimes \text{id} - 3(\chi_{3/2}(\hat{\nu}) + \hat{\nu}^{-1}\text{sgn}_{3/2}(\hat{\nu})) \otimes \hat{P} \right. \\ &\quad \left. + \frac{9}{2}\hat{\nu}^{-1}(\chi_{3/2}(\hat{\nu}) - \frac{1}{2}\hat{\nu}^{-1}\text{sgn}_{3/2}(\hat{\nu})) \otimes \hat{P}^2 + O(P^3/\bar{\nu}^3)\right) \end{aligned} \quad (52)$$

and

$$\begin{aligned} \hat{O}_c &= \frac{1}{2\sqrt{3}}i \left(\frac{1}{2}\gamma\ell_P^2\right)^{3/2} |\hat{\nu}| \left(2\Delta_3|\hat{\nu}|^{1/2} \otimes \text{id} + 3(\hat{\nu}^{-1}\Delta_3|\hat{\nu}|^{1/2} - \Delta_3(|\hat{\nu}|^{-1/2}\text{sgn}(\hat{\nu}))) \otimes \hat{P} \right. \\ &\quad \left. - \frac{9}{2}(\hat{\nu}^{-1}\Delta_3(|\hat{\nu}|^{-1/2}\text{sgn}(\hat{\nu})) + \frac{1}{2}\Delta_3|\hat{\nu}|^{-3/2}) \otimes \hat{P}^2 + O(P^3/\bar{\nu}^3)\right). \end{aligned} \quad (53)$$

where $\hat{\nu} = 6\hat{p}/(\gamma\ell_P^2)$ and $\hat{P} = 4\hat{p}_\varepsilon/(\gamma\ell_P^2)$. From these expressions we can read off the first coefficients $O_{A,\text{iso}}^{(k)}$ and $O_{c,\text{iso}}^{(k)}$.

Note that, while the expressions χ_δ , sgn_δ and Δ_δ can be directly extended to be applied to operators, the expansions are not densely defined on $\mathcal{H}_{\text{pert}}$ because of inverse powers of $\hat{\nu}$. In fundamental expressions where the classical analog has inverse powers of \hat{p} , such as matter Hamiltonians, one can still define densely defined operators [23, 24]. Here, however, we started with densely defined operators and obtained inverse powers only after expanding in the perturbative sector. We thus cannot change those terms and make them densely defined. For what follows we can mostly ignore this issue, disregarding states at small $\bar{\nu}$ on which the operators cannot be applied. We will come back to it in the discussion of singularities in Sec. 5.

Next we must have the action of the several terms to the left of \hat{O}_A and \hat{O}_c in (45). Up to order ε^3 we have

$$\begin{aligned} \hat{H} &= 4\pi^{-1}i\gamma^{-3}G^{-1}\ell_P^{-2} \left[2 \left\{ \sin^2 \frac{1}{2}\bar{c} \cos^2 \frac{1}{2}\bar{c} \otimes \text{id} + \frac{1}{2} \left(-\sin \frac{1}{2}\bar{c} \cos^3 \frac{1}{2}\bar{c} + \sin^3 \frac{1}{2}\bar{c} \cos \frac{1}{2}\bar{c} \right) \otimes \varepsilon \right. \right. \\ &\quad \left. \left. + \frac{1}{2} \left(-3 \sin^2 \frac{1}{2}\bar{c} \cos^2 \frac{1}{2}\bar{c} - \cos^4 \frac{1}{2}\bar{c} - \sin^4 \frac{1}{2}\bar{c} \right) \otimes \varepsilon^2 + \frac{1}{12} \left(\sin \frac{1}{2}\bar{c} \cos^3 \frac{1}{2}\bar{c} - \sin^3 \frac{1}{2}\bar{c} \cos \frac{1}{2}\bar{c} \right) \otimes \varepsilon^3 \right. \right. \\ &\quad \left. \left. + O(\varepsilon^4) \right\} \hat{O}_A + \right. \\ &\quad \left\{ \sin^2 \frac{1}{2}\bar{c} \cos^2 \frac{1}{2}\bar{c} \otimes \text{id} + \left(\sin \frac{1}{2}\bar{c} \cos^3 \frac{1}{2}\bar{c} - \sin^3 \frac{1}{2}\bar{c} \cos \frac{1}{2}\bar{c} \right) \otimes \varepsilon \right. \\ &\quad \left. + \frac{1}{4} \left(-6 \sin^2 \frac{1}{2}\bar{c} \cos^2 \frac{1}{2}\bar{c} + \cos^4 \frac{1}{2}\bar{c} + \sin^4 \frac{1}{2}\bar{c} \right) \otimes \varepsilon^2 + \frac{2}{3} \left(-\sin \frac{1}{2}\bar{c} \cos^3 \frac{1}{2}\bar{c} + \sin^3 \frac{1}{2}\bar{c} \cos \frac{1}{2}\bar{c} \right) \otimes \varepsilon^3 \right. \\ &\quad \left. \left. + O(\varepsilon^4) \right\} \hat{O}_c \right]. \end{aligned} \quad (54)$$

From (25), the relevant combinations of sines and cosines on the isotropic basis above have the matrix form

$$\begin{aligned}
\langle \bar{\nu} | \sin^2 \frac{1}{2} \bar{c} \cos^2 \frac{1}{2} \bar{c} | \bar{\mu} \rangle &= -2^{-4} (\delta_{\bar{\nu}, \bar{\mu}+4} - 2\delta_{\bar{\nu}, \bar{\mu}} + \delta_{\bar{\nu}, \bar{\mu}-4}), \\
\langle \bar{\nu} | \sin \frac{1}{2} \bar{c} \cos^3 \frac{1}{2} \bar{c} | \bar{\mu} \rangle &= -2^{-4} i (\delta_{\bar{\nu}, \bar{\mu}+4} + 2\delta_{\bar{\nu}, \bar{\mu}+2} - 2\delta_{\bar{\nu}, \bar{\mu}-2} - \delta_{\bar{\nu}, \bar{\mu}-4}), \\
\langle \bar{\nu} | \sin^3 \frac{1}{2} \bar{c} \cos \frac{1}{2} \bar{c} | \bar{\mu} \rangle &= 2^{-4} i (\delta_{\bar{\nu}, \bar{\mu}+4} - 2\delta_{\bar{\nu}, \bar{\mu}+2} + 2\delta_{\bar{\nu}, \bar{\mu}-2} - \delta_{\bar{\nu}, \bar{\mu}-4}), \\
\langle \bar{\nu} | \sin^4 \frac{1}{2} \bar{c} | \bar{\mu} \rangle &= 2^{-4} (\delta_{\bar{\nu}, \bar{\mu}+4} - 4\delta_{\bar{\nu}, \bar{\mu}+2} + 6\delta_{\bar{\nu}, \bar{\mu}} - 4\delta_{\bar{\nu}, \bar{\mu}-2} + \delta_{\bar{\nu}, \bar{\mu}-4}), \\
\langle \bar{\nu} | \cos^4 \frac{1}{2} \bar{c} | \bar{\mu} \rangle &= 2^{-4} (\delta_{\bar{\nu}, \bar{\mu}+4} + 4\delta_{\bar{\nu}, \bar{\mu}+2} + 6\delta_{\bar{\nu}, \bar{\mu}} + 4\delta_{\bar{\nu}, \bar{\mu}-2} + \delta_{\bar{\nu}, \bar{\mu}-4}). \quad (55)
\end{aligned}$$

So the total action in (54) is given by

$$\begin{aligned}
\langle \bar{\nu} | \hat{H} | \bar{\mu} \rangle &= \frac{1}{4\pi} i \gamma^{-3} G^{-1} \ell_P^{-2} \left\{ \delta_{\bar{\nu}, \bar{\mu}} \left[(4 - 18\varepsilon^2) \hat{O}_A(\bar{\nu}) + 2\hat{O}_c(\bar{\nu}) \right] \right. \\
&+ \delta_{\bar{\nu}, \bar{\mu}+4} \left[(-2 + 2i\varepsilon + \varepsilon^2) \hat{O}_A(\bar{\nu}) + (-1 - 2i\varepsilon + 2\varepsilon^2) \hat{O}_c(\bar{\nu}) \right] \\
&+ \left. \delta_{\bar{\nu}, \bar{\mu}-4} \left[(-2 - 2i\varepsilon + \varepsilon^2) \hat{O}_A(\bar{\nu}) + (-1 + 2i\varepsilon + 2\varepsilon^2) \hat{O}_c(\bar{\nu}) \right] + O(\varepsilon^3) \right\} \quad (56)
\end{aligned}$$

as matrix elements in \mathcal{H}_{iso} taking operator values in \mathcal{H}_S (for fixed $\bar{\nu}$, $\hat{O}_A(\bar{\nu})$ and $\hat{O}_c(\bar{\nu})$ are considered as operators on $|\bar{\nu}\rangle \otimes \mathcal{H}_S \cong \mathcal{H}_S$).

We can act with (56) on a generic state $|s\rangle = \sum_{\nu} s_{\nu}(\varepsilon) |\nu\rangle$ and use (52, 53). For this we write the Hamiltonian in the form

$$\langle \bar{\nu}, \varepsilon | \hat{H} | s \rangle = -\frac{1}{16\pi} \sqrt{\frac{3}{2}} G^{-1} \gamma^{-3/2} \ell_P \left\{ \hat{A}_{\bar{\nu}+4} s_{\bar{\nu}+4}(\varepsilon) + \hat{B}_{\bar{\nu}} s_{\bar{\nu}}(\varepsilon) + \hat{C}_{\bar{\nu}-4} s_{\bar{\nu}-4}(\varepsilon) \right\}, \quad (57)$$

where

$$\begin{aligned}
\hat{C}_{\bar{\nu}} &= -\frac{2}{3} (|\bar{\nu}|^{1/2} \text{sgn}_{3/2}(\bar{\nu}) + |\bar{\nu}| \Delta_3 |\bar{\nu}|^{1/2}) + \frac{2}{3} (|\bar{\nu}|^{1/2} \text{sgn}_{3/2}(\bar{\nu}) - 2|\bar{\nu}| \Delta_3 |\bar{\nu}|^{1/2}) i\varepsilon \\
&+ \left(\frac{2}{3} |\bar{\nu}|^{1/2} (\chi_{3/2}(\bar{\nu}) + \bar{\nu}^{-1} \text{sgn}_{3/2}(\bar{\nu})) - \text{sgn} \bar{\nu} \Delta_3 |\bar{\nu}|^{1/2} + |\bar{\nu}| \Delta_3 (|\bar{\nu}|^{-1/2} \text{sgn} \bar{\nu}) \right) \hat{P} \\
&+ \frac{3}{2} \left(-|\bar{\nu}|^{-1/2} \text{sgn} \bar{\nu} \chi_{3/2}(\bar{\nu}) + \frac{1}{2} |\bar{\nu}|^{-3/2} \text{sgn}_{3/2}(\bar{\nu}) + \text{sgn} \bar{\nu} \Delta_3 (|\bar{\nu}|^{-1/2} \text{sgn} \bar{\nu}) + \frac{1}{2} |\bar{\nu}| \Delta_3 |\bar{\nu}|^{-3/2} \right) \hat{P}^2 \\
&- (|\bar{\nu}|^{1/2} \chi_{3/2}(\bar{\nu}) + |\bar{\nu}|^{-1/2} \text{sgn} \bar{\nu} \text{sgn}_{3/2}(\bar{\nu}) + 2 \text{sgn} \bar{\nu} \Delta_3 |\bar{\nu}|^{1/2} - 2|\bar{\nu}| \Delta_3 (|\bar{\nu}|^{-1/2} \text{sgn} \bar{\nu})) i\varepsilon \hat{P} \\
&+ \frac{1}{3} (|\bar{\nu}|^{1/2} \text{sgn}_{3/2}(\bar{\nu}) + 4|\bar{\nu}| \Delta_3 |\bar{\nu}|^{1/2}) \varepsilon^2 + O(3), \quad (58)
\end{aligned}$$

$$\begin{aligned}
\hat{B}_{\bar{\nu}} &= \frac{4}{3} (|\bar{\nu}|^{1/2} \text{sgn}_{3/2}(\bar{\nu}) + |\bar{\nu}| \Delta_3 |\bar{\nu}|^{1/2}) \\
&- 2 (|\bar{\nu}|^{1/2} \chi_{3/2}(\bar{\nu}) + |\bar{\nu}|^{-1/2} \text{sgn} \bar{\nu} \text{sgn}_{3/2}(\bar{\nu}) - \text{sgn} \bar{\nu} \Delta_3 |\bar{\nu}|^{1/2} + |\bar{\nu}| \Delta_3 (|\bar{\nu}|^{-1/2} \text{sgn} \bar{\nu})) \hat{P} \\
&+ 3 (|\bar{\nu}|^{-1/2} \text{sgn} \bar{\nu} \chi_{3/2}(\bar{\nu}) - \frac{1}{2} |\bar{\nu}|^{-3/2} \text{sgn}_{3/2}(\bar{\nu}) - \text{sgn} \bar{\nu} \Delta_3 (|\bar{\nu}|^{-1/2} \text{sgn} \bar{\nu}) - \frac{1}{2} |\bar{\nu}| \Delta_3 |\bar{\nu}|^{-3/2}) \hat{P}^2 \\
&- 6|\bar{\nu}|^{1/2} \text{sgn}_{3/2}(\bar{\nu}) \varepsilon^2 + O(3) \quad (59)
\end{aligned}$$

and $\hat{A}_{\bar{\nu}} = \overline{\hat{C}_{\bar{\nu}}}$. Note that this is not the adjoint of $\hat{C}_{\bar{\nu}}$ but the complex conjugate (acting only on the numerical coefficients, not on possible factors of the imaginary unit in a derivative representation of \hat{P}). Complex conjugation and adjoint are not the same in this case because of the $\varepsilon \hat{P}$ -term. Also the whole constraint operator is not self-adjoint since we started with a non-symmetric ordering with holonomy operators to the left.

4 Evolution

The constraint equation given by the operator (57), i.e. requiring physical states to be annihilated by the constraint operator, results in a difference-differential equation for $s_n(\varepsilon)$ which can be interpreted as evolution equation in the volume $\bar{\nu}$ as internal time. This equation is difference-differential because we keep the underlying discreteness from quantum geometry in the isotropic variable, but treat the anisotropy perturbatively. Also in isotropic models one can have difference-differential equations if there is a matter degree of freedom such as a scalar, but the crucial difference here is that there are differential operators at all levels of the difference equation and in particular the leading ones. This has implications for the recurrence scheme since those operators have to be inverted in some manner. We perform here only a basic analysis to check if the scheme has satisfactory properties concerning evolution and relation to classical behavior.

We focus on the stability issue for which in our context three different notions occur. First, in the perturbative setting stability is already relevant at the classical level where one needs to make sure that anisotropies stay small enough for sufficiently long time. As can be seen from the discussion leading to (22), this can be ensured for some range of evolution at least in the vacuum case for our situation. The second notion is stability at the quantum level in the sense of [25], requiring that there are no exponentially growing solutions to the difference equation. This will be the focus in the following sections. Finally, also numerical stability issues can arise when difference or difference-differential equations are solved numerically.

We consider the evolution equation (57) without matter for large $\bar{\nu}$, for which the constraint equation reduces to

$$\begin{aligned} \frac{-\sqrt{3} \ell_{\text{P}}}{2^{3/2} \kappa \gamma^{3/2}} \left[\left(-\frac{4}{3} + \frac{4}{3}i\varepsilon + \frac{2}{3}\varepsilon^2 - \frac{6}{\bar{\nu}}i\varepsilon\hat{P} + \frac{3}{2\bar{\nu}^2}\hat{P}^2 \right) s_{\bar{\nu}+4}(\varepsilon) + \right. \\ \left. \left(-\frac{4}{3} - \frac{4}{3}i\varepsilon + \frac{2}{3}\varepsilon^2 + \frac{6}{\bar{\nu}}i\varepsilon\hat{P} + \frac{3}{2\bar{\nu}^2}\hat{P}^2 \right) s_{\bar{\nu}-4}(\varepsilon) + \right. \\ \left. \left(\frac{8}{3} - \frac{2}{\bar{\nu}}\hat{P} - 12\varepsilon^2 - \frac{3}{\bar{\nu}^2}\hat{P}^2 \right) s_{\bar{\nu}}(\varepsilon) \right] = 0 \end{aligned} \quad (60)$$

Now we propose a restricted function space for the solutions of the form

$$s_{\bar{\nu}}(\varepsilon) = p_{\bar{\nu}}^{(k)}(\varepsilon) e^{-(\varepsilon-\varepsilon_0)^2/4\sigma^2}, \quad (61)$$

where $p_{\bar{\nu}}^{(k)}$ are complex valued polynomials of order k . Since we expanded the Hamiltonian constraint to second order, we also should disregard terms of higher order in the solutions and work with $k = 2$. Then,

$$p_{\bar{\nu}}^{(2)}(\varepsilon) = A_0(\bar{\nu}) + A_1(\bar{\nu}) \varepsilon + A_2(\bar{\nu}) \varepsilon^2 \quad (62)$$

where A_0 , A_1 and A_2 are complex valued functions of the discrete time $\bar{\nu}$ only, to be determined from initial values through the difference equation. This class of functions is

general enough for our purposes because, even though ε_0 and σ are fixed, the Gaussian can be deformed and spread if A_1 and A_2 grow as functions of $\bar{\nu}$. Moreover, to the given order of expansion also non-zero expectation values for \hat{p}_ε are allowed through complex valued A_1 and A_2 . For a Gaussian state peaked at anisotropy p_ε^0 we need a phase factor $e^{6i\varepsilon p_\varepsilon^0/\gamma\ell_P^2}$ which for small enough p_ε^0 can be expanded, only contributing imaginary parts to A_1 and A_2 . For this, we need to assume $p_\varepsilon^0 \ll \ell_P^2$ which is possible but not guaranteed by our general perturbation assumptions. Still, for the tests we are going to perform such small values are sufficient. For more detailed aspects one has to generalize the allowed class of functions.

Computing (60) using $\hat{P} = -\frac{2}{3}id/d\varepsilon$ and (61), (62) for large $\bar{\nu}$, and collecting terms of the same order in ε we obtain

$$\begin{aligned} & A_0(\bar{\nu} + 4) (2\sigma^2 - 8\bar{\nu}^2\sigma^4 - \varepsilon_0^2) - 2A_0(\bar{\nu}) (2\sigma^2 - 8\bar{\nu}^2\sigma^4 - 2i\bar{\nu}\sigma^2\varepsilon_0 - \varepsilon_0^2) \\ & \quad + A_0(\bar{\nu} - 4) (2\sigma^2 - 8\bar{\nu}^2\sigma^4 - \varepsilon_0^2) \\ & + A_1(\bar{\nu} + 4) (-4\sigma^2\varepsilon_0) - 2A_1(\bar{\nu}) (-4i\bar{\nu}\sigma^4 - 4\sigma^2\varepsilon_0) + A_1(\bar{\nu} - 4) (-4\sigma^2\varepsilon_0) \\ & \quad + A_2(\bar{\nu} + 4) (-8\sigma^4) - 2A_2(\bar{\nu}) (-8\sigma^4) + A_2(\bar{\nu} - 4) (-8\sigma^4) = 0 \end{aligned} \quad (63)$$

from leading order in ε ,

$$\begin{aligned} & A_0(\bar{\nu} + 4) (8i\bar{\nu}^2\sigma^4 - 12\bar{\nu}\sigma^2\varepsilon_0 + 2\varepsilon_0) - 2A_0(\bar{\nu}) (-2i\bar{\nu}\sigma^2 + 2\varepsilon_0) \\ & \quad + A_0(\bar{\nu} - 4) (-8i\bar{\nu}^2\sigma^4 + 12\bar{\nu}\sigma^2\varepsilon_0 + 2\varepsilon_0) \\ & + A_1(\bar{\nu} + 4) (6\sigma^2 - 24\bar{\nu}\sigma^4 - 8\bar{\nu}^2\sigma^4 - \varepsilon_0^2) - 2A_1(\bar{\nu}) (6\sigma^2 - 8\bar{\nu}^2\sigma^4 - \varepsilon_0^2 - 2i\bar{\nu}\sigma^2\varepsilon_0) \\ & \quad + A_1(\bar{\nu} - 4) (6\sigma^2 + 24\bar{\nu}\sigma^4 - 8\bar{\nu}^2\sigma^4 - \varepsilon_0^2) \\ & + A_2(\bar{\nu} + 4) (-8\sigma^2\varepsilon_0) - 2A_2(\bar{\nu}) (-8i\bar{\nu}\sigma^4 - 8\sigma^2\varepsilon_0) + A_2(\bar{\nu} - 4) (-8\sigma^2\varepsilon_0) = 0 \end{aligned} \quad (64)$$

from linear order, and

$$\begin{aligned} & A_0(\bar{\nu} + 4) (-1 + 12\bar{\nu}\sigma^2 + 4\bar{\nu}^2\sigma^4) - 2A_0(\bar{\nu}) (-1 + 36\bar{\nu}^2\sigma^4) \\ & \quad + A_0(\bar{\nu} - 4) (-1 - 12\bar{\nu}\sigma^2 + 4\bar{\nu}^2\sigma^4) \\ & + A_1(\bar{\nu} + 4) (8i\bar{\nu}^2\sigma^4 + 2\varepsilon_0 - 12\bar{\nu}\sigma^2\varepsilon_0) - 2A_1(\bar{\nu}) (2i\bar{\nu}\sigma^2 + 2\varepsilon_0) \\ & \quad + A_1(\bar{\nu} - 4) (-8i\bar{\nu}^2\sigma^4 + 2\varepsilon_0 + 12\bar{\nu}\sigma^2\varepsilon_0) \\ & + A_2(\bar{\nu} + 4) (10\sigma^2 - 48\bar{\nu}\sigma^4 - 8\bar{\nu}^2\sigma^4 - \varepsilon_0^2) - 2A_2(\bar{\nu}) (10\sigma^2 - 8\bar{\nu}^2\sigma^4 - 2i\bar{\nu}\sigma^2\varepsilon_0 - \varepsilon_0^2) \\ & \quad + A_2(\bar{\nu} - 4) (10\sigma^2 + 48\bar{\nu}\sigma^4 - 8\bar{\nu}^2\sigma^4 - \varepsilon_0^2) = 0 \end{aligned} \quad (65)$$

from quadratic order. As the equations are quite complicated, we discuss here mainly their approximation for large volume which can already be used to see relations to the classical behavior.

4.1 Asymptotic $\bar{\nu}$ solution

While the perturbation scheme does not require a relation between the magnitudes of $\bar{\nu}$ and ε_0 or $\sigma \sim \varepsilon_0 \ll 1$, for a given choice of ε_0 and σ consistent with the perturbation

assumptions we can look at the asymptotic form of the equations where only highest powers of $\bar{\nu}$ are used. For the second order equations, this requires $\bar{\nu} \gg \sigma^{-2}$ which is our assumption for the asymptotic regime. Simplifying the equations then leads to

$$\begin{aligned}
A_0(\bar{\nu} + 4) - 2A_0(\bar{\nu}) + A_0(\bar{\nu} - 4) &= 0, \\
A_1(\bar{\nu} + 4) - 2A_1(\bar{\nu}) + A_1(\bar{\nu} - 4) &= i [A_0(\bar{\nu} + 4) - A_0(\bar{\nu} - 4)], \\
A_2(\bar{\nu} + 4) - 2A_2(\bar{\nu}) + A_2(\bar{\nu} - 4) &= \frac{1}{2} [A_0(\bar{\nu} + 4) - 18A_0(\bar{\nu}) + A_0(\bar{\nu} - 4)] + \\
&\quad i [A_1(\bar{\nu} + 4) - A_1(\bar{\nu} - 4)]. \tag{66}
\end{aligned}$$

We can already observe that, in contrast to (63), these equations are independent of the value of ε_0 in complete analogy to our previous observation for the asymptotic classical solution (22). Also, the equations have imaginary terms which is necessary for p_ε to change in internal time (in the ε -representation chosen here, p_ε enters through the phase of the wave function). Even if p_ε^0 is initially zero, i.e. A_0 , A_1 and A_2 are all real, the wave function must become complex after some steps such that anisotropy also in the triad arises automatically.

Before solving (66) we generalize it to allow dust like matter (matter Hamiltonian independent of $\bar{\nu}$) such that the middle coefficients on the left hand sides of the equations are 2ρ with a constant $\rho \leq 1$, reproducing the vacuum case above for $\rho = 1$. We then put the system in a first order form, considering solutions only on the lattice $4\mathbb{Z}$ which is sufficient to see the behavior of long-time evolution. Accordingly, we introduce the vector

$$\mathbf{v}(\bar{\nu} + 4) = \begin{pmatrix} A_0(\bar{\nu} + 4) \\ A_1(\bar{\nu} + 4) \\ A_2(\bar{\nu} + 4) \\ A_0(\bar{\nu}) \\ A_1(\bar{\nu}) \\ A_2(\bar{\nu}) \end{pmatrix}.$$

With this definition we can cast (66) in a first-order linear matrix equation (of stepsize four):

$$M \mathbf{v}(\bar{\nu} + 4) + N \mathbf{v}(\bar{\nu}) = \mathbf{0} \quad \text{or} \quad \mathbf{v}(\bar{\nu} + 4) + Q \mathbf{v}(\bar{\nu}) = \mathbf{0}, \tag{67}$$

where the matrix Q is

$$Q = \begin{pmatrix} -2\rho & 0 & 0 & 1 & 0 & 0 \\ -2i\rho & -2\rho & 0 & 2i & 1 & 0 \\ 9 + \rho & 2i\rho & -2\rho & -2 & 2i & 1 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \end{pmatrix}.$$

It is possible to bring this matrix to its Jordan canonical form (see App. B) $J = S^{-1}QS$ where

$$J = \begin{pmatrix} \lambda_1 & 1 & 0 & 0 & 0 & 0 \\ 0 & \lambda_1 & 1 & 0 & 0 & 0 \\ 0 & 0 & \lambda_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_2 & 1 & 0 \\ 0 & 0 & 0 & 0 & \lambda_2 & 1 \\ 0 & 0 & 0 & 0 & 0 & \lambda_2 \end{pmatrix}.$$

Here, $\lambda_{1,2} = \pm\sqrt{\rho^2 - 1} - \rho$ are the two eigenvalues of Q with multiplicity three (which degenerate further in the vacuum case $\rho = 1$).

From here we can obtain the solution starting from initial conditions in (67):

$$\mathbf{v}(\bar{\nu}_0 + 4k) = Q^k \mathbf{v}(\bar{\nu}_0). \quad (68)$$

We obtain

$$Q^k = S J^k S^{-1}, \quad (69)$$

where J is the Jordan form for Q above and each one of its block powers is

$$J_i^k = \sum_{j=0}^2 \binom{k}{j} \lambda_i^{k-j} N^j. \quad (70)$$

N is the off-diagonal term in J .

We obtain the transition matrix S by computing the generalized eigenvectors associated to $\lambda_{1,2}$, which we do not write down; however we write the general k -power of J above:

$$J^k = \begin{pmatrix} \lambda_1^k & k\lambda_1^{k-1} & \binom{k}{2}\lambda_1^{k-2} & 0 & 0 & 0 \\ 0 & \lambda_1^k & k\lambda_1^{k-1} & 0 & 0 & 0 \\ 0 & 0 & \lambda_1^k & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_2^k & k\lambda_2^{k-1} & \binom{k}{2}\lambda_2^{k-2} \\ 0 & 0 & 0 & 0 & \lambda_2^k & k\lambda_2^{k-1} \\ 0 & 0 & 0 & 0 & 0 & \lambda_2^k \end{pmatrix}.$$

From this the solution for the A functions is

$$A_0(\bar{\nu}_0 + 4k) = \frac{1}{2}(\rho^2 - 1)^{-1/2} ((-\lambda_1^k \lambda_2 + \lambda_1 \lambda_2^k) A_0(\bar{\nu}_0) + (\lambda_2^k - \lambda_1^k) A_0(\bar{\nu}_0 - 4)), \quad (71)$$

$$A_1(\bar{\nu}_0 + 4k) = \frac{1}{2}(\rho^2 - 1)^{-1/2} ((-\lambda_1^k \lambda_2 + \lambda_1 \lambda_2^k) A_1(\bar{\nu}_0) - ik(-\lambda_1^2 \lambda_2^{k-1} + \lambda_1^{k-1} \lambda_2^2) A_0(\bar{\nu}_0) + i(\lambda_2^k - \lambda_1^k - k\lambda_1^{k-1} \lambda_2 + k\lambda_2^{k-1} \lambda_1) A_0(\bar{\nu}_0 - 4) (\lambda_2^k - \lambda_1^k) A_1(\bar{\nu}_0 - 4)) \quad (72)$$

and

$$\begin{aligned}
A_2(\bar{\nu}_0 + 4k) &= \frac{1}{4} \left[\frac{9}{(\rho^2 - 1)^{3/2}} (\lambda_1^k - \lambda_2^k) \right. \\
&+ k\lambda_1^{k-1} \left(\frac{-9 - 2\rho + 18\rho^2 + 2\rho^3}{\rho^2 - 1} + \frac{-1 + 18\rho + 2\rho^2}{\sqrt{\rho^2 - 1}} \right) \\
&+ \binom{k}{2} \frac{2\lambda_1^{k-2}}{\rho^2 - 1} (1 - 5\rho^2 + 4\rho^4 - 3\rho\sqrt{\rho^2 - 1} + 4\rho^3\sqrt{\rho^2 - 1}) \\
&+ k\lambda_2^{k-1} \left(\frac{-9 - 2\rho + 18\rho^2 + 2\rho^3}{\rho^2 - 1} + \frac{-1 + 18\rho + 3\rho^2 + 18\rho^3 - 2\rho^4}{(\rho^2 - 1)^{3/2}} \right) \\
&+ \binom{k}{2} \lambda_2^{k-2} \left(\frac{2 - 12\rho^2 + 18\rho^4 - 8\rho^6}{(\rho^2 - 1)^2} + \frac{6\rho - 14\rho^3 + 8\rho^5}{(\rho^2 - 1)^{3/2}} \right) \Big] A_0(\bar{\nu}_0) \\
&- \frac{ik}{2} \left(\frac{\lambda_1^{k-1}\lambda_2^2 - \lambda_2^{k-1}\lambda_1}{\sqrt{\rho^2 - 1}} \right) A_1(\bar{\nu}_0) + \frac{1}{2} \left(\frac{-\lambda_1^k\lambda_2 + \lambda_2^k\lambda_1}{\sqrt{\rho^2 - 1}} \right) A_2(\bar{\nu}_0) \\
&+ \frac{1}{4} \left[\lambda_1^k \frac{1 - 9\rho + \rho^2}{(\rho^2 - 1)^{3/2}} + \lambda_2^k \frac{1 + 9\rho - \rho^2}{(\rho^2 - 1)^{3/2}} \right. \\
&+ 3k \left(-\lambda_1^{k-1} \left\{ 1 + \frac{3\rho}{\rho^2 - 1} + \frac{3 + \rho}{\sqrt{\rho^2 - 1}} \right\} + \lambda_2^{k-1} \left\{ -1 - \frac{3\rho}{\rho^2 - 1} + \frac{3 + \rho}{\sqrt{\rho^2 - 1}} \right\} \right) \\
&+ \binom{k}{2} \left(\lambda_1^{k-2} \left\{ 4\rho + 2\frac{2\rho^2 - 1}{\sqrt{\rho^2 - 1}} \right\} \right. \\
&+ \left. \lambda_2^{k-2} \left\{ \frac{4\rho}{(\rho + 1)^2} - 2\frac{2\rho^2 - 1}{(\rho + 1)^{3/2}\sqrt{\rho - 1}} \right\} \right) \Big] A_0(\bar{\nu}_0 - 4) \\
&+ \frac{i}{2} \left(\frac{\lambda_2^k - \lambda_1^k}{(\rho^2 - 1)^{\frac{3}{2}}} - k\frac{\lambda_1^{k-1}\lambda_2 - \lambda_1\lambda_2^{k-1}}{\sqrt{\rho^2 - 1}} \right) A_1(\bar{\nu}_0 - 4) \\
&+ \frac{\lambda_2^k - \lambda_1^k}{2\sqrt{\rho^2 - 1}} A_2(\bar{\nu}_0 - 4). \tag{73}
\end{aligned}$$

This solution is valid only for $|\rho| \neq 1$, for otherwise the eigenvalues would be completely degenerate.

So we have obtained the solution to the evolution equation in the asymptotic $\bar{\nu}$ regime. We should note that the solutions grow as powers of the order k (no larger than second) as a consequence of degeneracy, although the leading coefficient A_0 is bounded.

4.2 Inclusion of matter

One can hope that matter terms remove the degeneracy present for the case for pure gravity, which similarly happens in the isotropic model (see [11] for an explicit isotropic

vacuum solution which is also unbounded). As the previous discussion shows however, this is not the case for dust which has a constant diagonal Hamiltonian, $\hat{H} = E\mathbb{I}$.

As the next simple possibility we can consider a cosmological constant term

$$\hat{H}_{\text{matter}} = \Lambda \hat{V}. \quad (74)$$

Using (48) the evolution equation for large $\bar{\nu}$ (60) modifies to

$$\begin{aligned} & \left(-\frac{4}{3} + \frac{4}{3}i\varepsilon + \frac{2}{3}\varepsilon^2 - \frac{6}{\bar{\nu}}i\varepsilon\hat{P} + \frac{3}{2\bar{\nu}^2}\hat{P}^2 \right) s_{\bar{\nu}+4} + \\ & \left(-\frac{4}{3} - \frac{4}{3}i\varepsilon + \frac{2}{3}\varepsilon^2 + \frac{6}{\bar{\nu}}i\varepsilon\hat{P} + \frac{3}{2\bar{\nu}^2}\hat{P}^2 \right) s_{\bar{\nu}-4} + \\ & \left(\frac{8}{3} - \frac{2}{\bar{\nu}}\hat{P} - 12\varepsilon^2 - \frac{3}{\bar{\nu}^2}\hat{P}^2 \right) s_{\bar{\nu}} = \\ & -\frac{4}{3}\pi G\gamma^3\Lambda \left(\frac{2\bar{\nu}^{3/2}}{3} - \frac{9}{4\sqrt{\bar{\nu}}}\hat{P}^2 \right) s_{\bar{\nu}}. \end{aligned} \quad (75)$$

With the same ansatz (61), (62) the right hand side of each equation becomes

$$\frac{\bar{\nu}^{3/2}}{6} [A_0(\bar{\nu})(54\sigma^2 + 32\bar{\nu}^2\sigma^4 - 27\varepsilon_0^2) + A_1(\bar{\nu})(-108\sigma^2\varepsilon_0) + A_2(\bar{\nu})(-216\sigma^4)] \quad (76)$$

for (63),

$$\frac{\bar{\nu}^{3/2}}{6} [A_0(\bar{\nu})(54\varepsilon_0) + A_1(\bar{\nu})(162\sigma^2 + 32\bar{\nu}^2\sigma^4 - 27\varepsilon_0^2) + A_2(\bar{\nu})(-216\sigma^2\varepsilon_0)]$$

for (64) and

$$\frac{\bar{\nu}^{3/2}}{6} [A_0(\bar{\nu})(-27) + A_1(\bar{\nu})(54\varepsilon_0) + A_2(\bar{\nu})(270\sigma^2 + 32\bar{\nu}^2\sigma^4 - 27\varepsilon_0^2)]$$

for (65).

It is easier to check the degeneracy in the asymptotic $\bar{\nu}$ regime: in this case the right hand sides of (66) acquire an extra term $\frac{27}{9}\pi G\gamma^3\Lambda\bar{\nu}^{3/2}A_i(\bar{\nu})$, respectively. Coefficients in the asymptotic difference equation are thus no longer constant and we do not find explicit solutions. Still, around any fixed $\bar{\nu}$ eigenvalues remain degenerate.

4.3 Large $\bar{\nu}$ behavior

Rather than looking at more involved matter choices, we now use only large $\bar{\nu}$ and keep next order terms in $\bar{\nu}^{-1}$. This gives rise to more complicated correction terms in (63) compared to the asymptotic equations, changing all coefficients. Rather than trying to solve this second order system of difference equations, we perform a local stability analysis around large fixed $\bar{\nu}$ similar to that in the previous section

To this end we put the system (60) again in a first order form (67), where now the matrices $\mathbf{M}, \mathbf{N}, \mathbf{Q}$ are functions of $(\bar{\nu}, \varepsilon_0, \sigma)$. In this case the stability of the system is obtained if and only if the module of the eigenvalues of the matrix \mathbf{Q} above are less or equal to one. However its characteristic polynomial is of order six and, recalling the form of (63), each one of its coefficients is a very complex function of $(\bar{\nu}, \varepsilon_0, \sigma)$. Therefore we perform a numerical analysis to see the behavior of each one of the coefficient functions $A_i(\bar{\nu})$ in (62).

The characteristic polynomial is of the form

$$\begin{aligned} \lambda^6 + h_5 \lambda^5 + h_4 \lambda^4 + h_3 \lambda^3 + h_2 \lambda^2 + h_1 \lambda + h_0 &= 0, \\ h_j &= h_j(\bar{\nu}, \varepsilon_0, \sigma), \quad j = 0 \dots 5 \end{aligned} \tag{77}$$

which one can solve numerically to find choices of ε_0 and σ where all six roots have an absolute value less than or equal to one.

5 Perturbations and the singularity

When perturbing in basic variables, the expansion is valid only for $p_\varepsilon \ll \bar{p}$ and thus breaks down very close to the classical singularity. Indeed, the main aim for studying perturbations is to understand effects in structure formation where one needs at least perturbative inhomogeneities for which anisotropies serve as a model. This is usually modelled in semiclassical regimes, in an inflationary phase or sometimes through a bounce at relatively large volume, far away from the Planck scale. It is nevertheless instructive to discuss implications for the singularity issue itself close to vanishing \bar{p} , as they might appear in a perturbative setting.

In the asymptotic $\bar{\nu}$ equation (66) we saw that the relevant matrix M in (67) at highest order of the difference equation is always invertible such that evolution cannot break down in this regime. But this is not guaranteed at small $\bar{\nu}$ where a breakdown of evolution can occur even at $\bar{\nu} > 0$ where one would not expect singularities classically. There are even divergences in coefficients of the difference equation such as in $\hat{C}_{\bar{\nu}}$ for $\bar{\nu} = 3$ coming, e.g., from $\Delta_3 |\bar{\nu}|^{-3/2}$. This is certainly a small value for $\bar{\nu}$, but note that p_ε can be small compared to \bar{p} even for $\bar{\nu}$ of the order one which perturbatively is consistent using the fact that the perturbative operator p_ε has a continuous spectrum. As discussed earlier, small p_ε do not automatically bring us into discrete regimes, unlike small \bar{p} . One can thus set up the perturbative evolution such that all assumptions for the perturbation scheme are satisfied, and yet the evolution breaks down at non-zero volume. (Starting at large volume, the perturbative approximation is expected to break down much before the classical singularity is reached. But generically, a breakdown of evolution cannot be ruled out since there are initial conditions for which the evolution breaks down *before* the perturbative scheme ceases to make sense.)

There is thus no removal of singularities in the perturbative model. Even worse, the perturbative equation could make us believe that the non-singular evolution of the isotropic model is very special and could not extend to less symmetric models, owing to the fact that

for $\varepsilon = P = 0$ all divergent coefficients disappear. In such a situation, it is necessary to use the full model from which the perturbative equation is derived in order to see whether or not it breaks down. As it turns out, for loop quantum cosmology the evolution is non-singular even for anisotropic models, in contrast to the perturbative appearance.

A different source for a breakdown of evolution appears because coefficients of the difference equation are now differential operators on the perturbative degree of freedom. These operators must be inverted to proceed with the evolution, which is not generically possible and may require special boundary conditions. Note that, if a physical inner product is not known, even generic invertibility would not be enough: one needs to make sure that any initial state can be evolved without breakdown to conclude singularity freedom. Even if almost all initial values would lead to non-singular evolution, all of them could be ruled out by the physical inner product (see also [6]). We do not discuss this in detail here but only conclude that, while the fully quantized anisotropic model is non-singular, there is no such statement in the perturbative quantization.

It is interesting to compare this situation with recent results in string theory [26] where inhomogeneities on a background are seen to prevent the occurrence of a bounce instead of a singularity (which would otherwise be possible in the corresponding homogeneous model). This looks similar to our perturbative quantization of anisotropies on an isotropic background, even though the models and techniques are certainly very different. In contrast, non-perturbative background independent models studied so far are non-singular, including inhomogeneous ones which classically have local physical degrees of freedom [27].

There is a further disadvantage of using perturbative or semiclassical degrees of freedom in order to discuss the singularity issue, as for instance suggested in [28]. Such a perturbative treatment is unlikely to remain valid close to a singularity where potentially all degrees of freedom can be excited strongly. Perturbations certainly allow one to include all degrees of freedom which is important for phenomenology, but properties of the singularity can be extremely blurred as we have seen here. In contrast, symmetric models completely remove many degrees of freedom which may have to be reinserted later on when discussing their effect on evolution. But symmetric models themselves are often classically singular, and those singularities can be studied by quantizations of models. With the models now available, the most characteristic types of classical singularities can be studied also at the quantum level. This can then show how classical singularities can be resolved by quantization, and there is indeed a general mechanism in loop quantum gravity.

While the fundamental singularity issue concerning the extension of solutions to the Hamiltonian constraint equation cannot be analyzed perturbatively, this is still possible for phenomenological models of bounces as studied in [29] and used for the construction of oscillatory universe models in [30]. Such bounces need to happen sufficiently far above the Planck scale in order to ensure the validity of effective equations [31], and thus avoid a potential breakdown of the perturbative discrete evolution. This will also be true for perturbative analyses of inhomogeneities. Also at the inhomogeneous level, one can employ approximate but non-perturbative methods in the spirit of the BKL picture [32]. In contrast to perturbative schemes, this can then also be applied to the fundamental singularity issue, as done in the loop quantum gravity context with preliminary investigations in [33].

6 Conclusions

We have mainly illustrated the reduction procedure to symmetric situations available for loop quantum gravity, and contrasted it with a new method for perturbative quantum degrees of freedom in the case of anisotropy. We consider this mainly as a model situation for the cosmologically more interesting but technically much more complicated case of perturbative inhomogeneities. This already allowed us to draw some cautionary conclusions for the singularity problem when discussed in a perturbative setting, as well as for the relation between symmetric models and perturbative less symmetric ones.

The resulting evolution equations are of a new type compared to other models in loop quantum gravity. Although not studied in detail here, they are treatable at least by numerical schemes and provide an interesting setting to understand evolution equations in general and numerical techniques to solve them. New schemes for an efficient solution still need to be developed, also taking into account the issue of pre-classicality [34] ignored here. This condition requires solutions not to vary strongly on the scale of discreteness. It can be expected for semiclassical behavior, but is also necessary to ensure the correct behavior of wave packets. Techniques to extract pre-classical solutions, such as those based on generating functions [35], continued fractions [36] or numerical ones using suitable function bases [37], have been introduced but are not yet available for the equations considered here.

Also the equations themselves can be generalized in several directions. Within the same degree of symmetry one can discuss different matter choices and, at the level of the ansatz (61), more general classes for the functional behavior of the wave function depending on anisotropy. Moreover, different orderings of the constraint operator, most importantly the symmetric one, can be tried. The bigger step consists in including inhomogeneous degrees of freedom perturbatively for which the analysis in this paper serves as preparation. Classically, the split into symmetric and non-symmetric variables would be given by a mode decomposition with respect to the symmetric background. A priori, there are no insurmountable difficulties in repeating the analysis here for this situation, even though technically it would be much more involved. Inhomogeneities can already be included explicitly by using midi-superspace models for which the loop framework has been constructed in [18, 38]. These situations already allow the inclusion of inhomogeneities of cosmological interest.

Our analysis also shows that the reduced constraint of the more symmetric model still plays a role for the less symmetric one and is only amended by perturbative correction terms. Those terms are derived by expanding the less symmetric constraint operator, and not by quantizing the classically expanded constraint in the fashion of [39]. Indeed, the additional terms are much more contrived than expected classically. Although more complicated, these terms are derived from the less-symmetric model and are thus well-motivated. After a detailed study of the evolution, such as restrictions from quantum stability, one can draw conclusions for the form of the less symmetric constraint operator. (Such restrictions indeed arise easily as the closed isotropic model, [10] compared to [40], and the more detailed analysis in [25] showed.) Eventually, with a better understanding of the relation between models and the full theory also at the level of the Hamiltonian

constraint, one can then hope to restrict possible full constraint operators and reduce their ambiguities.

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Appendix

A Approximate action of operators on peaked states

For the perturbative expansion of the Hamiltonian constraint at the quantum level it is necessary to define and discuss an appropriate notion of expansions of operators. We are not interested in expansions valid for any state of the Hilbert space but only in expansions that can be used for states corresponding to small anisotropy such as those used in (61). Thus, the expansion parameter is not contained directly in the original operator but introduced through a restricted class of states considered for the action. We then start by choosing a space \mathcal{D}_δ of states in the original Hilbert space \mathcal{H} , or even a subset of a cylindrical space Cyl_S , depending on the intended perturbation parameter δ (or several ones such as ε_0 and p_ε^0 in the main part of this paper, and define

Definition 1 *An operator \hat{O}_k on \mathcal{H} is an approximation of order k to an operator \hat{O} if $\hat{O}_k\Psi$ agrees, with respect to the inner product, with $\hat{O}\Psi$ for all $\Psi \in \mathcal{D}_\delta$ up to order δ^{k+1} , i.e.*

$$\langle \Psi' | (\hat{O} - \hat{O}_k) \Psi \rangle = O(\delta^{k+1})$$

for all $\Psi' \in \text{Cyl}_S$. Agreement with respect to the inner product in this sense will be denoted by $\hat{O}_k\Psi \sim \hat{O}\Psi$.

To show that this is realized for the expansions performed for anisotropies in this paper, we choose \mathcal{D}_{q_0, p^0} to be the span of states of the form $\Psi(q) = \sigma^{-1/2} s(q) \exp(-(q - q_0)^2/4\sigma^2) \exp(ip^0 q)$ for a given $\sigma < q_0$ and a polynomial s (we do not normalize states but keep track of factors of σ). Expansions performed here always lead to approximations \hat{O}_k which are polynomials in the basic operators \hat{q} and \hat{p} of the anisotropy. This implies that any \hat{O}_k considered here maps the space \mathcal{D}_δ to itself and can be used to show that the validity of expansions is preserved by taking products:

Lemma 1 Let $\hat{O}_k^{(1)}$ and $\hat{O}_k^{(2)}$ be approximations of $\hat{O}^{(1)}$ and $\hat{O}^{(2)}$, respectively, such that they fix the spaces \mathcal{D}_δ and Cyl_S . Then $\hat{O}_k^{(1)}\hat{O}_k^{(2)}$ is an approximation of $\hat{O}^{(1)}\hat{O}^{(2)}$.

Proof: By assumption we have $\hat{O}^{(1)}\hat{O}^{(2)}\Psi \sim \hat{O}^{(1)}\hat{O}_k^{(2)}\Psi$ because we can simply replace Ψ' by $\hat{O}^{(1)\dagger}\Psi'$ in the definition of agreement. Since $\hat{O}_k^{(2)}\Psi$ is in \mathcal{D}_δ for $\Psi \in \mathcal{D}_\delta$, we have

$$\hat{O}^{(1)}\hat{O}^{(2)}\Psi \sim \hat{O}_k^{(1)}\hat{O}_k^{(2)}\Psi$$

which finishes the proof. \square

We can therefore split the expansion into different steps as done in the main calculations here. This also simplifies the proof that the performed expansion of the Hamiltonian constraint is an approximation because we only need to show that multiplication operators can be approximated by simply expanding the multiplying function, which we would apply for our calculations in both the coordinate and momentum representation. We then only need

Lemma 2 Let $\hat{O}\Psi(q) = O(q)\Psi(q)$ be a multiplication operator on $\hat{H} = L^2(\mathbb{R}, dq)$. Any partial Taylor sum $O_k(q) = \sum_{n=0}^k \frac{1}{n!}O^{(n)}(0)q^n$ gives rise to an approximation $\hat{O}_k\Psi(q) = O_k(q)\Psi(q)$ of \hat{O} order k with respect to \mathcal{D}_δ as above.

Proof: Let $\Psi(q) = \sigma^{-1/2}s(q)\exp(-(q - q_0)^2/4\sigma^2)$ and $\Psi' \in \text{Cyl}_S$. We have

$$\begin{aligned} |\langle \Psi' | (\hat{O} - \hat{O}_k) \Psi \rangle| &= \sigma^{-1/2} \left| \int dq \bar{\Psi}'(q) (O(q) - O_k(q)) s(q) \exp(-(q - q_0)^2/4\sigma^2) \right| \\ &\leq 2C_1 \sigma^{-1/2} \int_{q_0}^{q_0+1} \exp(-(q - q_0)^2/4\sigma^2) q^{k+1} dq \\ &\quad + 2C_2 \sigma^{-1/2} \int_{q_0+1}^{\infty} \exp(-(q - q_0)^2/4\sigma^2) q^{k+1} dq \end{aligned}$$

with positive constants C_1 and C_2 depending only on the supremum of the real and imaginary parts of $\bar{\Psi}'(q)s(q)$. The first integral can be estimated by

$$\begin{aligned} \int_{q_0}^{q_0+1} \exp(-(q - q_0)^2/4\sigma^2) q^{k+1} dq &= \int_0^1 \exp(-q^2/4\sigma^2) (q + q_0)^{k+1} dq \\ &= \sigma^{k+2} \int_0^{\sigma^{-1}} \exp(-q^2/4) (q + q_0/\sigma)^{k+1} dq \\ &\leq \sigma^{k+2} \int_0^{\infty} \exp(-q^2/4) (q + q_0/\sigma)^{k+1} dq \end{aligned}$$

where the last integral exists and does not depend strongly on q_0 and σ since they are assumed to be of the same order. The whole expression is thus of order σ^{k+2} . For the

second integral, we have

$$\begin{aligned} \int_{q_0+1}^{\infty} \exp(-(q - q_0)^2/4\sigma^2)q^{k+1}dq &= e^{-(2\sigma)^{-2}} \int_0^{\infty} \exp(-(q^2 + 2q)/4\sigma^2)(q + q_0 + 1)^{k+1}dq \\ &\leq e^{-(2\sigma)^{-2}} \int_0^{\infty} \exp(-q^2/4\sigma^2)(q + 2)^{k+1}dq \end{aligned}$$

where the last integral is a polynomial in σ and the whole expression is thus of the order $e^{-(2\sigma)^{-2}}$ times a polynomial in σ . By our assumptions on the states in \mathcal{D}_σ , we have σ of the order or smaller than q_0 which concludes the proof. \square

B Jordan canonical form

B.1 Generalized eigenvectors and transition matrix

In this section we briefly review the Jordan canonical form of a square complex matrix. For further details and the proofs of the theorems see for example [41]. We begin stating the following

Theorem 1 *If a square matrix A of order n has s linearly independent eigenvectors, then it is similar to a matrix J of the following form, called a Jordan canonical form*

$$J = S^{-1}AS = \begin{pmatrix} J_1 & & & 0 \\ & J_2 & & \\ & & \ddots & \\ 0 & & & J_s \end{pmatrix}, \quad (78)$$

in which each J_i , called the Jordan block, is a triangular matrix of the form

$$J_i = \begin{pmatrix} \lambda_i & 1 & & 0 \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ 0 & & & \lambda_i \end{pmatrix}, \quad (79)$$

where λ_i is a single eigenvalue of A . Each Jordan block corresponds to a linearly independent eigenvector.

This theorem states that we can bring any square matrix to its Jordan form. The usefulness of this form lies in the fact that it is easier to obtain powers of the matrix A , as can be seen by taking a look at the form of J in (78), (79). The matrix S in (78) is called the *transition matrix*. Now we state the procedure to obtain both matrices J and S .

The basic elements to obtain the Jordan form are the *generalized eigenvectors*, replacing ordinary eigenvectors of a diagonalizable matrix.

Definition 2 A nonzero vector \mathbf{x} is said to be a generalized eigenvector of A of rank k belonging to an eigenvalue λ if

$$(A - \lambda I)^k \mathbf{x} = \mathbf{0} \quad \text{and} \quad (A - \lambda I)^{k-1} \mathbf{x} \neq \mathbf{0}. \quad (80)$$

If $k = 1$ this is the usual definition of an eigenvector. For a generalized eigenvector \mathbf{x} of rank larger than one belonging to the eigenvalue λ define

$$\begin{aligned} \mathbf{x}_k &= \mathbf{x}, \\ \mathbf{x}_{k-1} &= (A - \lambda I)\mathbf{x} = (A - \lambda I)\mathbf{x}_k, \\ \mathbf{x}_{k-2} &= (A - \lambda I)^2\mathbf{x} = (A - \lambda I)\mathbf{x}_{k-1}, \\ &\vdots \\ \mathbf{x}_2 &= (A - \lambda I)^{k-2}\mathbf{x} = (A - \lambda I)\mathbf{x}_3, \\ \mathbf{x}_1 &= (A - \lambda I)^{k-1}\mathbf{x} = (A - \lambda I)\mathbf{x}_2. \end{aligned} \quad (81)$$

One can check that each one of the \mathbf{x}_j above is a generalized eigenvector of the eigenvalue λ .

Definition 3 The set of vectors $\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$ is called a chain of generalized eigenvectors belonging to the eigenvalue λ .

Now the transition matrix S can be constructed from the chains of linearly independent generalized eigenvectors of A [41].

B.2 Powers of square matrices

The Jordan canonical form of any square matrix A enables us to compute its powers A^k . Let J be the Jordan canonical form of an arbitrary $n \times n$ matrix A such that

$$S^{-1}AS = J = \begin{pmatrix} J_1 & & \\ & \ddots & \\ & & J_s \end{pmatrix},$$

where S is made of the generalized eigenvectors of A and J_s are Jordan blocks.

Since we have

$$A^k = S^{-1}J^kS = S \begin{pmatrix} J_1^k & & \\ & \ddots & \\ & & J_s^k \end{pmatrix} S^{-1}$$

for $k = 1, 2, \dots$, it is enough to compute J^k for each Jordan block J . An $m \times m$ Jordan block J belonging to an eigenvalue λ of A may be written as

$$J = \begin{pmatrix} \lambda & 1 & & 0 \\ 0 & \ddots & \ddots & \\ & & \lambda & 1 \\ 0 & & 0 & \lambda \end{pmatrix} = \lambda \mathbb{I}_{m \times m} + \begin{pmatrix} 0 & 1 & \cdots & 0 \\ 0 & \ddots & \ddots & 0 \\ \vdots & & 0 & 1 \\ 0 & \cdots & 0 & 0 \end{pmatrix} = \lambda \mathbb{I} + N,$$

where \mathbb{I} is the identity matrix and N is nilpotent. Clearly we have

$$J^k = (\lambda\mathbb{I} + N)^k = \sum_{j=0}^k \binom{k}{j} \lambda^{k-j} N^j. \quad (82)$$

But $N^k = 0$ for $k \geq m$ and thus, by defining $\binom{k}{l} = 0$ if $k < l$

$$\begin{aligned} J^k &= \sum_{j=0}^{m-1} \binom{k}{j} \lambda^{k-j} N^j \\ &= \lambda^k \mathbb{I} + k\lambda^{k-1}N + \dots + \binom{k}{m-1} \lambda^{k-(m-1)} N^{m-1}. \end{aligned} \quad (83)$$

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