Quantum Cosmological Backreactions III: Deparametrised Quantum Cosmological Perturbation Theory

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Abstract

This is the third paper in a series of four in which we use space adiabatic methods in order to incorporate backreactions among the homogeneous and between the homogeneous and inhomogeneous degrees of freedom in quantum cosmological perturbation theory.

In this paper we consider a particular kind of cosmological perturbation theory which starts from a gauge fixed version of General Relativity. The gauge fixing is performed using a material reference system called Gaussian dust. The resulting system has no constraints any more but possesses a physical Hamiltonian that drives the dynamics of both geometry and matter. As observable matter content we restrict to a scalar field (inflaton). We then explore the sector of that theory which is purely homogeneous and isotropic with respect to the geometry degrees of freedom but contains inhomogeneous perturbations up to second order of the scalar field.

The purpose of this paper is to explore the quantum field theoretical challenges of the space adiabatic framework in a cosmological model of inflation which is technically still relatively simple. We compute the quantum backreaction effects from every energy band of the inhomogeneous matter modes on the evolution of the homogeneous geometry up to second order in the adiabatic parameter. These contributions turn out to be significant due to the infinite number of degrees of freedom and are very sensitive to the choice of Fock representation chosen for the inhomogeneous matter modes.

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Contents

1 Introduction 3
2 The Hamiltonian 4
3 Space Adiabatic Perturbation Scheme 5
  3.1 Parameter-Dependent Harmonic Oscillators 5
  3.2 Structural Ingredients 6
  3.3 Construction of the Moyal Projector $\pi^{(b,p_b)}_{n}$ 7
  3.4 Construction of the Moyal Unitary $u^{(b,p_b)}_{n}$ 8
  3.5 Construction of the Effective Hamiltonian $h^{(b,p_b)}_{eff,n}$ 9
4 Conclusion and Outlook 11
1 Introduction

In a previous paper of this series [1] we have emphasised the importance of an adequate description of backreaction effects between homogeneous and inhomogeneous degrees of freedom and between geometry and matter in quantum cosmology [2]. We have argued that the framework of space adiabatic perturbation theory (SAPT) [3] is ideally suited to do this because it is able to combine the framework of quantum field theory on curved classical spacetimes (QFT in CST) [5] with the fundamental quantum nature of that background. The way this works is quite similar to the quantum field theory on non-commutative spacetimes approach of [6] where Weyl quantisation techniques are used in order to employ the ordinary QFT framework while spacetime coordinates are non-commutative. Here, instead of the spacetime coordinates we use Weyl quantisation techniques in order to treat a non-commutative quantum background. Here the homogeneous degrees of freedom play the role of the “slow” degrees of freedom while the inhomogeneous ones are “fast”.

However, SAPT not only harmonically synthesises the apparently contradicting natures of the background geometry in quantum cosmology on the one hand and QFT in CST on the other but also provides a concrete scheme for how to systematically compute backreaction effects between the homogeneous quantum background geometry and the inhomogeneous quantum matter and quantum geometry. The separate treatment of the homogeneous and inhomogeneous degrees of freedom of a quantum field is called the hybrid scheme [7] which we adopt in this series of papers. Moreover, the SAPT scheme can also deal with the situation that the coupling between the slow and fast degrees of freedom depends on both, configuration and momentum variables, of the slow sector which goes beyond what one can do in a Born-Oppenheimer approach [8]. More generally, it is able to treat the situation that the slow sector couples with mutually non-commuting operators. As emphasised in [9], this is very important when one goes beyond cosmological perturbation theory and tries to quantise geometry with the methods of Loop Quantum Gravity (LQG) [10] while matter is quantised using the QFT in CST framework because in LQG even the spatial geometry to which matter fields couple becomes non-commutative.

In this paper we consider General Relativity coupled to an inflaton field as well as Gaussian dust [11]. We use the dust fields to deparametrise the theory [12] so that all geometry degrees of freedom (scalar, vector, tensor) and the inflaton become (Dirac) observables and the theory is equipped with a true conservative Hamiltonian which for Gaussian dust is particularly simple: it is nothing but the gravitational and inflaton contribution to the Hamiltonian constraint integrated over space. One can then apply classical cosmological perturbation theory to this system in the fashion outlined in all detail in [13] for a different material reference system [14]. For the illustrative purpose of this paper we discard the inhomogeneous geometry degrees of freedom and focus on the homogeneous geometry and homogeneous and inhomogeneous inflaton sector to second order in the inhomogeneities. Note that the inhomogeneous field species decouple to second order. We reserve the treatment of inhomogeneous geometry degrees of freedom to our fourth paper [15]. This artificial restriction serves the purpose of mathematical convenience: We would like to illustrate the SAPT formalism in a cosmological, quantum field theoretical context which is as simple as possible in order not to get lost in details that have nothing to do with the SAPT programme itself. We stress that the inhomogeneous geometry modes can be treated by exactly the same methods.

The application of the SAPT scheme to this quantum field theoretical model in principle proceeds just like the purely homogeneous quantum mechanical model [4] with two important differences: First, it is absolutely crucial that one first applies a canonical transformation (ex-
act up to second order in the inhomogenous perturbations) to this system in order to switch to variables which have the property that in terms of them the background dependent Fock representations of the inflaton all employ the same Hilbert space for every background. This is otherwise not the case as observed in [9] where the very same model was considered and which would then prevent the application of the SAPT scheme. In [9] therefore an artificial cut-off on the number of degrees of freedom had to be introduced. That this can be avoided by means of a transformation which mixes homogeneous and inhomogeneous degrees of freedom was first observed in [16] in a different context. Second, it is necessary to perform a further canonical transformation in the homogeneous sector in order to avoid the problems that come from tachyonic quantum fields [1]. After these subtleties have been dealt with, we proceed as in [4] and compute the second order correction (with respect to the adiabatic parameter, to be distinguished from the order with respect to the inhomogeneous perturbations) to the inhomogeneous dynamics from every energy band of the inhomogeneous sector. This adiabatic correction is highly non-trivial and is quite sensitive to the Fock representation chosen in the inhomogeneous sector: If not carefully selected, the adiabatic correction can easily diverge. These findings have potentially observational consequences since they should influence the details of the quantum cosmological bounce observed for instance in Loop Quantum Cosmology (LQC) [17] which describes the truncation of LQG to the homogeneous sector without backreactions.

The architecture of this paper is as follows:

In section two we briefly introduce the model and prepare it for the application of the SAPT scheme by performing the afore mentioned field truncations and canonical transformations. In section three we then directly apply the SAPT framework. We assume the reader to be familiar with the notation and main formulae of [1]. The obtained adiabatic corrections display a rather singular character with respect to the homogeneous degrees of freedom, however, the corresponding operator has, in the Schrödinger representation, the computationally convenient dense and invariant domain of [18]. In section four we summarise and conclude.

2 The Hamiltonian

The Hamiltonian, after a transformation which is canonical up to second order in the cosmological perturbations (see [1] for more details), includes an effective mass term \( M^2 \) which for arbitrary phase space variables \( (a, p_a) \) needs not to be positive definite. As already commented in [1], a possible solution for this, is to perform a canonical transformation to new cosmological variables \( (b, p_b) \), given by,

\[
a = \sqrt{b^2 + \sigma^2 \frac{p_b^2}{b^2}} =: \Sigma^{(b,p_b)}, \quad p_a = a \cdot \frac{p_b}{b}.
\]

In order to not confuse the different sets of variables, we defined the scale factor \( a \) as a function of \( (b, p_b) \) as \( \Sigma \). According to space adiabatic perturbation theory, the symbol Hamiltonian which serves for the analysis in the sequel is thus given by,

\[
\mathcal{H} = \mathcal{L}^3 \left( -\frac{1}{12} \frac{\Sigma^{(b,p_b)}_{,b}^2}{b^2} + \Lambda \Sigma^3 \right) \mathbf{1}_{\mathcal{K}} + \frac{1}{2 \Sigma} \int_{\mathcal{T}^3} d^3x \left( \frac{\pi^2}{\sqrt{\phi h}} + \sqrt{\phi h} \phi \left( -\Delta + \mu^2 b^2 \right) \right),
\]

\[
= \mathcal{E}_{\mathcal{G}}^{(b,p_b)} \mathbf{1}_{\mathcal{K}} + \frac{1}{2 \Sigma} \int_{\mathcal{T}^3} d^3x \left( \frac{\pi^2}{\sqrt{\phi h}} + \sqrt{\phi h} \phi \left( -\Delta + \mu^2 b^2 \right) \right),
\]

(2)
where the space manifold is assumed to be a compact three-torus $\mathbb{T}^3$ with volume $L^3$. The commutation relations for the new cosmological pair and for the scalar field are,

$$\left[\hat{b}, \hat{p}_b\right]_c = \frac{i\varepsilon}{L^3} \hat{1}_c, \quad [\phi, \pi]_{\text{KG}} = i \hat{1}_{\text{KG}}$$

(3)

For the compact model, a Fourier transform with discrete Fourier modes for the Klein-Gordon system is at our disposal. Since the space adiabatic scheme requires the choice of an (arbitrary) discrete energy value of the Klein-Gordon system, it is self-evident to pass over to the mode description. Furthermore, we employ a particle description for the Klein-Gordon field i.e., expressing the Hamiltonian by means of creation- and annihilation operators for each Fourier mode. The Hamiltonian symbol is then given by,

$$h = E^{(b,p_b)}_G 1_{\text{KG}} + \frac{1}{\sum_{\kappa \in \Theta} \omega^{(b)}_{\kappa}} \sum_{\kappa \in \Theta} \omega^{(b)}_{\kappa} (a^{(b)}_{\kappa})^\dagger a^{(b)}_{\kappa}$$

(4)

where $\omega^{(b)}_{\kappa} := \sqrt{k^2 + \mu^2 b^2}$, and $\Theta := \frac{2\pi}{\ell} (\mathbb{Z}^3 \backslash \{0\})$. The annihilation and creation operators satisfy the commutation relations,

$$\left[ a^{(b)}_{\kappa}, (a^{(b)}_{\kappa'})^\dagger \right]_{\text{KG}} = \delta_{\kappa,\kappa'} 1_{\text{KG}},$$

(5)

where $\delta_{\kappa,\kappa'}$ is the Kronecker delta. The $b$-dependence of the creation- and annihilation operators will be examined in the next section. The representation of the commutation relations will be chosen as the tensor product, $\mathcal{H}_G \otimes \mathcal{H}_{\text{KG}}$. The first factor is a simple $L^2$-space over the real axis with Lebesgue measure $db$, while the second factor is the symmetric Fock space $\mathcal{F}_s(\ell^2(\Theta))$ with respect to the one particle Hilbert space $\ell^2(\Theta)$ of the discrete Fourier modes (counting measure understood).

3 Space Adiabatic Perturbation Scheme

3.1 Parameter-Dependent Harmonic Oscillators

We examine the characteristics of the Hamilton symbol, (2). The eigenvalue problem of the parameter-dependent Hamilton operator $h^{(b,p_b)}$ for the Klein-Gordon subsector has the form,

$$h^{(b,p_b)} e^{(b)}_{n_d} = E^{(b,p_b)} e^{(b)}_{n_d}.$$

(6)

Here, $n_d$ is a short form for the number of excitations $n_{\kappa,d}$ for every wavenumber $\kappa$ and for the degeneracy label $d \in \{1,...,D\}$, where $D$ is the multiplicity of the eigenenergy $E^{(b,p_b)}_n$. The $D$ degenerate eigensolutions $e^{(b)}_{n_d}(b)$ are mutually orthonormal. The energy value is explicitly given by,

$$E^{(b,p_b)}_n = E^{(b,p_b)}_G + E^{(b,p_b)}_{\text{KG},n} = E^{(b,p_b)}_G + \frac{1}{\sum_{\kappa \in \Theta} \omega^{(b)}_{\kappa} n_{\kappa,d}} \sum_{\kappa \in \Theta} \omega^{(b)}_{\kappa} n_{\kappa,d}.$$  

(7)

The corresponding eigenstates are derived from the vacuum state $\Omega^{(b)} \in \mathcal{F}_s(\ell^2(\Theta))$ as follows,

$$e^{(b)}_{n_d} = \prod_{\kappa \in \Theta} \left( (a^{(b)}_{\kappa})^\dagger \right)^{n_{\kappa,d}} \frac{\sqrt{n_{\kappa,d}!}}{\Omega^{(b)}}.$$

(8)
For the procedure of space adiabatic perturbation theory, we choose one particular eigenenergy $E_{n}^{(b,p)}$ and we denote the corresponding $b$-dependent projector as,

$$\pi_{n,b}^{(b)} := \sum_{d=1}^{D} \varepsilon_{n,d}^{(b)} \langle e_{n,d}^{(b)} , \cdot \rangle_{\mathcal{K}G}$$

where $\langle \cdot , \cdot \rangle_{\mathcal{K}G} : F_{s}(\mathcal{E}^{2}(\Theta)) \times F_{s}(\mathcal{E}^{2}(\Theta)) \to \mathbb{C}$ denotes the inner product of the Klein-Gordon Hilbert space. Since we restrict the application to one particular, albeit arbitrary, eigenband with quantum number(s) $n_{\tilde{m},d, \tilde{k}} \in \Theta$, we omit the index $n$ for the Moyal projector in what follows, i.e., we write $\pi_{0}^{(b)} := \pi_{a,b}^{(b)}$ instead.

The space adiabatic scheme uses the derivatives of the eigensolutions $e_{n,d}^{(b)}$ with respect to the gravitational canonical pair. Since the eigensolutions do not depend on the momentum, $p_{\epsilon}$, it suffices to compute the $b$-derivative of $e_{n,d}^{(b)}$. Similar to the simple quantum mechanical models in [4], it can be shown that, on the one hand, the $b$-derivative separately decreases the excitation number by two, for any wave number $\tilde{m}$ which is already excited at least twice, i.e., for which $n_{\tilde{m},d} \geq 2$. On the other hand, the $b$-derivative separately increases the excitation number by two for every wave number $\tilde{m}$. The twofold lowered and raised states enter with the respective factors,

$$\alpha_{1,n_{\tilde{m}},d}^{(b)} := -f^{(b)} \frac{\sqrt{(n_{\tilde{m},d-1}+\tilde{m},d)}}{2}, \quad \alpha_{2,n_{\tilde{m}},d}^{(b)} := -f^{(b)} \frac{\sqrt{(n_{\tilde{m},d+1}+\tilde{m},d+2)}}{2},$$

where the function $f^{(b)}$ is defined via the frequency,

$$f^{(b)} := -\frac{1}{2} \frac{\partial \ln(\omega_{k}^{(b)})}{\partial b}.$$  

Hereby, the $b$-derivative of $e_{n,d}^{(b)}$ is given by,

$$\frac{\partial e_{n,d}^{(b)}}{\partial b} = \sum_{\tilde{m} \in \Theta} \prod_{\tilde{k} \in \Theta} \alpha_{1,n_{\tilde{m}},d}^{(b)} \left( a^{(b)}_{\tilde{k}} \right)^{n_{\tilde{m},d}+2} \sqrt{(n_{\tilde{m},d})!} + \alpha_{2,n_{\tilde{m}},d}^{(b)} \left( a^{(b)}_{\tilde{k}} \right)^{n_{\tilde{m},d}+2} \sqrt{(n_{\tilde{m},d+2})!} \right) \Omega^{(b)}$$

$$= \sum_{\tilde{m} \in \Theta} \left( \alpha_{1,n_{\tilde{m}},d}^{(b)} \psi_{\{\cdots,n_{\tilde{m},d-2},\cdots\}}^{(b)} + \alpha_{2,n_{\tilde{m}},d}^{(b)} \psi_{\{\cdots,n_{\tilde{m},d+2},\cdots\}}^{(b)} \right),$$

where $e_{\{\cdots,n_{\tilde{m},d+2},\cdots\}}^{(b)}$ denotes the state which is raised, respectively lowered, in the quantum number $n_{\tilde{m},d}$ by two compared to $e_{n,d}^{(b)}$.

### 3.2 Structural Ingredients

Space adiabatic perturbation theory requires three structural conditions from the model in order to be applicable.

1. The quantum Hilbert space of the system decomposes as a tensor product,

$$\mathcal{H} = \mathcal{H}_{\epsilon} \otimes \mathcal{H}_{\mathcal{K}G},$$

and the dynamics in $\mathcal{H}_{\epsilon}$ happens on much larger scales as compared to the dynamics in $\mathcal{H}_{\mathcal{K}G}$. In this model, $\epsilon := \sqrt{\kappa/\lambda}$ represent the separation of these scales of change. As argued in [1], this result is in line with the separation of the homogeneous degrees of freedom and the non-homogeneous field variables within the model.
2. Deformation quantization with the Weyl ordering is employable for the quantization of the homogeneous cosmological subsystem. This makes space adiabatic perturbation theory work on a technical level.

3. The principal symbol of the Hamiltonian $\hat{h}^{(b,p_b)}$, which is already the total Hamiltonian symbol for this model, has a pointwise isolated part of the spectrum $\pi^{(b,p_b)}_{\epsilon}$. We choose one of the eigenspaces with energy label $\{n_{\vec{k},d}\}$, $\vec{k} \in \Theta$. For fixed and distinct variables $(b, p_b)$ an arbitrary shift in the quantum number(s) $n_{\vec{k},d}$ produces a distinct energy value.

In the following, we work out the details of the space adiabatic scheme, which consists in,

1) the construction of the Moyal projector, $\pi^{(b,p_b)}_n \in S^\infty(\epsilon; \Gamma_\epsilon, \mathcal{L}(\mathcal{H}_\epsilon))$

2) the construction of the Moyal unitary, $u^{(b,p_b)} \in S^\infty(\epsilon; \Gamma_\epsilon, \mathcal{L}(\mathcal{H}_\epsilon))$, and

3) the construction of the effective Hamiltonian, $h^{(b,p_b)}_{\text{eff}} \in S^\infty(\epsilon; \Gamma_\epsilon, \mathcal{L}(\mathcal{H}_\epsilon))$.

3.3 Construction of the Moyal Projector $\pi^{(b,p_b)}_n$

Space adiabatic perturbation theory rests on the space adiabatic theorem [3], which states that it is possible to construct iteratively a projection operator $\Pi_{(\epsilon)}$ of the full Hilbert space $\mathcal{H}$ up to order $\epsilon$ in the adiabatic perturbation parameter $\epsilon$, such that the subspace $\Pi_{(\epsilon)} \mathcal{H}$ is invariant under the evolution generated by the full Hamiltonian $\hat{h}$. For further information on the scheme and first intuitive examples, we refer the reader to [REF, REF]. Here, we only state that space adiabatic perturbation theory suggests to construct the above projection operator on the symbol level, with the projection operator, as the zeroth order starting point of the iterative construction scheme. The full Moyal projection operator has then the form of a formal perturbation series in $\epsilon$,

$$\pi^{(b,p_b)}_n := \sum_{d=1}^{D} \sum_{N=0}^{\infty} \varepsilon^N \pi^{(b,p_b)}_{n_{d},N}, \quad \pi^{(b,p_b)}_{n_{d},N} \in S^\infty(\Gamma_\epsilon, \mathcal{L}(\mathcal{F}_\epsilon(\ell^2(\Theta)))),$$

and we recall that the index $n_{d}$ is a set of excitations number associated to the degeneracy label $d$. The index $n$ is then the shortcut for the set of all these excitations number for all degeneracy labels.

As explained more in detail in [4, 1], the iterative conditions for the $N$-th order projection symbol, $\pi^{(b,p_b)}_{n_{N}}$, are given by,

1) $\pi^{(b,p_b)}_{(N)} \ast_\epsilon \pi^{(b,p_b)}_{(N)} - \pi^{(b,p_b)}_{(N)} = \mathcal{O}(\varepsilon^{N+1})$,

2) $\left(\pi^{(b,p_b)}_{(N)}\ast_\epsilon\right)^* - \pi^{(b,p_b)}_{(N)} = \mathcal{O}(\varepsilon^{N+1})$,

3) $[\hat{h}, \pi^{(b,p_b)}_{(N)}]_{\ast_\epsilon} = \mathcal{O}(\varepsilon^{N+1})$,

where "$\ast_\epsilon$" is the star product for the Weyl ordering, i.e., the pull back of the operator Weyl ordered multiplication on the space of semiclassical symbols. It is then straightforward to compute the first order contribution $\pi^{(b,p_b)}_{n,1}$ by means of the conditions [1] [2] [3] and the zeroth order projector, [4]. Thereby, we define the energy associated to a single excitation with respect to the mode $\vec{k}$ as, $\Delta_{\vec{k},d} := \omega^{(b)}_{\vec{k}} / \Sigma$. As a shorthand notation, we denote the eigenstate $\psi^{(b)}_{\{\ldots n_{\vec{k},d}^2, \ldots\}}$, which is raised, respectively lowered in the quantum number $n_{\vec{k},d}$ by
two compared to \( e_{n_d}^{(d)} \), by \( e_{n_d+2}^{(d)} \). Then, the contribution of first order to the Moyal projector is given by,

\[
\pi_1 = \frac{i}{2L^2} \sum_{d=1}^{D} \sum_{k \in \Theta} \left( \alpha_{1,n_{k,d}}^{(b)} E_{1,n_{k,d}}^{(b,p_d)} \left( e_{n_{k,d}}^{(b)} \langle e_{n_{k,d}+2}^{(b)}, \cdot \rangle - e_{n_{k,d}+2}^{(b)} \langle e_{n_{k,d}}, \cdot \rangle \right) 
+ \alpha_{2,n_{k,d}}^{(b)} E_{2,n_{k,d}}^{(b,p_d)} \left( e_{n_{k,d}}^{(b)} \langle e_{n_{k,d}+2}^{(b)}, \cdot \rangle - e_{n_{k,d}+2}^{(b)} \langle e_{n_{k,d}}, \cdot \rangle \right) \right)
\]

where we defined the \( n \)-dependent functions,

\[
E_{1,n_{k,d}}^{(b,p_d)} := \left( \frac{1}{\Delta_{E,k}} \left( \frac{\partial E_G}{\partial p_b} - \frac{1}{\sum \partial p_b} E_{KG,n} \right) + \frac{1}{\sum \partial p_b} \right),
\]

\[
E_{2,n_{k,d}}^{(b,p_d)} := \left( \frac{1}{\Delta_{E,k}} \left( \frac{\partial E_G}{\partial p_b} - \frac{1}{\sum \partial p_b} E_{KG,n} \right) + \frac{1}{\sum \partial p_b} \right),
\]

with \( E_G, E_{KG,n} \) and \( \Sigma \) respectively defined in (2), (7) and (1). We emphasize that the Weyl quantization of the projector \( \pi_{(1)}^{(b,p_d)} \) projects on a subspace of the full Hilbert space which is \( \varepsilon \)-dependent, and the description of the dynamics therein is non-trivial. Space adiabatic perturbation theory therefore suggests to construct a Moyal unitary symbol \( u_{(b,p_d)} \in S^\infty(\varepsilon; \Gamma_c, \mathcal{L}(\mathcal{F}_0(\ell^2(\Theta)))) \) which maps the dynamics of \( \pi^{(b,p_d)} \) to a suitable reference space \( \mathcal{H}_o \). This is the aim of the next section.

### 3.4 Construction of the Moyal Unitary \( u_{(b,p_d)} \)

For the given model, the simplest and physically most convenient choice of a reference space for projecting the dynamics from \( \mathcal{H}_{KG,n}^{(b,p_d)} := \pi_{(1)}^{(b,p_d)} \mathcal{H}_{KG} \) on, is given by taking \( \pi_{(1)}^{(b)} \mathcal{H}_{KG} \) for one particular \( b = b_0 \). In this section, we denote it as \( \mathcal{H}_0 \). The corresponding “reference” projector in \( \mathcal{H}_{KG} \) will be denoted by,

\[
\pi_0 := \sum_{d=1}^{D} e_{n_d}^{(b)} \langle e_{n_d}^{(b)}, \cdot \rangle_{KG}
\]

In order to mediate between \( \mathcal{H}_{KG}^{(b)} \) and \( \mathcal{H}_0 \), and vice versa, a unitary operator \( u_0 \) is necessary. The condition of unitarity and the requirement that \( u_0 \) should map \( \pi_0 \) to \( \pi_{(1)} \) gives at least the following conditions on \( u_0 \),

1) \( u_0 \cdot \pi_0 \cdot (u_0)^* = \pi_{(1)} \),

2) \( u_0 \cdot (u_0)^* = 1_{\mathcal{H}_0} \),

3) \( (u_0)^* \cdot u_0 = 1_{KG} \).

Therefore, we employ for \( u_0 \) the following operator-valued symbol,

\[
u_{(b)} = \sum_{j \geq 0} e_{j,b}^{(b)} \langle e_{j,b}^{(b)}, \cdot \rangle_{KG},
\]

where the index \( j \) is a short notation for the set of all possible excitation configurations within the Fock space \( \mathcal{F}_0(\ell^2(\Theta)) \). This choice trivially satisfies the conditions on \( u_0 \) and is simple and evident.
Taking \( u_0 \) and the above conditions as a starting point, we aim to construct iteratively a semiclassical symbol \( u_{n_d}^{(b,p_b)} \in S^\infty(\varepsilon; \Gamma_G, \mathcal{L}(\mathcal{H}_KG)) \). The formal power series has the form,

\[
u_{n_d}^{(b,p_b)} = \sum_{N \geq 0} \varepsilon^N u_{n_d, N}^{(b,p_b)}, \quad u_{n_d, N}^{(b,p_b)} \in S^\infty(\mathcal{L}(\mathcal{H}_KG)).\tag{21}
\]

Transcription of the conditions for \( u_0 \), the first order in \( \varepsilon \), gives for the semiclassical symbol \( u \in S^\infty(\varepsilon; \Gamma_G, \mathcal{L}(\mathcal{H}_KG)) \),

1) \( u \ast \pi \ast u^* = \pi_R \)
2) \( u \ast u^* - 1_{\mathcal{H}_0} = \mathcal{O}(\varepsilon^{N+1}) \)
3) \( (u) \ast u = 1_{\mathcal{H}_G} \).

Like for the Moyal projector, the perturbative equations for \( u \) read, when considered order by order in \( \varepsilon \),

1) \( u_{(N)} \ast \pi \ast (u_{(N)})^* - \pi_R = \mathcal{O}(\varepsilon^{N+1}) \),
2) \( u_{(N)} \ast (u_{(N)})^* - 1_{\mathcal{H}_0} = \mathcal{O}(\varepsilon^{N+1}) \),
3) \( (u_{(N)}) \ast u_{(N)} - 1_{\mathcal{H}_G} = \mathcal{O}(\varepsilon^{N+1}) \).

Since for the computation of the effective Hamilton symbol of second order, only the first order of the unitary symbol is necessary, we restrict our analysis to the computation of \( u_{(b,p_b)}^{(b,p_b)} \).

Given \( u_0 \), it is straightforward to show that the hermitian part of \( u_1 \) vanishes because \( u_0 \) is independent of \( p_b \). The remaining anti-hermitian part is given by,

\[
u_1 = \frac{i}{2 \mathcal{L}^2} \sum_{d=1}^D \sum_{k \in \Theta} \left( \alpha_{1,n_d,k}^{(b)} E_{1,n_d,k}^{(b,p_b)} (e_{n_d}^{(b)} (e_{n_d}^{(b)} - 2, \cdot) + e_{n_d}^{(b)} (e_{n_d}^{(b)} - 2, \cdot)) \right) \tag{22}
\]

\[
+ \alpha_{2,n_d,k}^{(b)} E_{2,n_d,k}^{(b,p_b)} (e_{n_d}^{(b)} (e_{n_d}^{(b)} + 2, \cdot) + e_{n_d}^{(b)} (e_{n_d}^{(b)} + 2, \cdot)) \right) \tag{23}
\]

### 3.5 Construction of the Effective Hamiltonian \( h_{eff,n}^{(b,p_b)} \)

The last step of the perturbation scheme consists in pulling the dynamics of the chosen subspace to the \( \varepsilon \)-independent subspace, \( \mathcal{H}_0 = \Pi_R \mathcal{H} \). This essentially means that by applying the unitary operator \( \hat{u} \) which is the Weyl quantization on the Hamiltonian \( \hat{h} \), the action of the latter on elements in \( \Pi \mathcal{H} \) is rotated to \( \mathcal{H}_0 \). We denote the semiclassical symbol,

\[
h_{eff} := u \ast \pi \ast (u)^*, \tag{24}
\]

as the effective Hamiltonian. Then, the Weyl quantization, \( \hat{h}_{eff} \), of the symbol \( h_{eff} \in S^\infty(\varepsilon; \Gamma_G, \mathcal{L}(\mathcal{H}_KG)) \) is essentially self-adjoint on the Schwartz space \( S(\mathbb{R}, \mathcal{H}_KG) \). And in particular, the dynamics of \( \hat{h} \) are mapped unitarily to \( \mathcal{H}_0 \), such that,

\[
\left[ \hat{h}_{eff}, \pi_R \right] = 0, \tag{25}
\]

\[
e^{-i\hat{h}_{eff} s} - (\hat{u})^* e^{-i\hat{h}_{eff} s} \hat{u} = \mathcal{O}(\varepsilon^\infty |s|), \tag{26}
\]
where $s \in \mathbb{R}$ is a real parameter.

We construct $h_{\text{eff}}$ perturbatively by means of equation (24) up to second order. We assume for the generic form of the semiclassical symbol $h_{\text{eff}},$

$$h_{\text{eff}}^{(b,p_b)} = \sum_{N \geq 0} \epsilon^N h_{\text{eff},N}^{(b,p_b)}, \quad h_{\text{eff},N}^{(b,p_b)} \in S^\infty(\Gamma_G, L(\mathcal{H}_{KG})) \quad (27)$$

Its restriction up to the $N$-th order, $h_{\text{eff},(N)}$, is defined as,

$$h_{\text{eff},(N)} = u_{(N)} \star h_{(N)} \star (u_{(N)})^* + \mathcal{O}(\epsilon^{N+1}). \quad (28)$$

Since we are mainly interested in the effective dynamics within the chosen subspace associated to $\pi_R$, we directly restrict the effective Hamilton symbol on this subspace by multiplying our results for $h_{\text{eff},(2)}$ by $\pi_R$ from the left and the right. We denote the latter symbol then by $h_{\text{eff},(n,(2))}$.

At zeroth order of the perturbation theory, the effective Hamilton symbol is then given by,

$$h_{\text{eff},n,0} = \pi_R \cdot u_0 \cdot h \cdot u_0^* \cdot \pi_R \quad (29)$$

$$= \left( L^3 \left( -\frac{1}{12} \sum_{\ell \in \Theta} \frac{p_\ell^2}{b^2} + \Lambda \Sigma^3 \right) + \frac{1}{\Sigma} \sum_{k \in \Theta} \omega_k^{(b)} n_{E,k} \right) \pi_R. \quad (30)$$

This corresponds to the Born-Oppenheimer adiabatic limit of the perturbation theory in which the effective Hamiltonian for the gravitational degrees of freedom not only contains the first "bare" gravitational part $E_G^{(b,p_b)}$, but also the backreaction contribution from the Klein-Gordon energy band $n_{E,k}$ that has been chosen.

The first order effective Hamilton symbol $h_{\text{eff},n,1}$, which can be computed straightforwardly using (25) together with the result for $h_{\text{eff},n,0}$, has no contribution within the chosen subspace. However, the generic effective Hamiltonian symbol does not vanish and it enters in the computation of the next order effective Hamiltonian symbol contribution. The space adiabatic perturbation scheme yields a priori for the second order contribution of the effective Hamiltonian,

$$h_{\text{eff},n,2} = \sum_{d=1}^{D} \left( \sum_{n_0 \in \Theta} \left( \frac{E_{\text{eff},d}^{(b,p_b)}}{\omega_m^{(b)}} \right)^3 \left( n_{m,d} + \frac{1}{2} \right) + \frac{E_{\text{eff},d}^{(b,p_b)}}{\omega_m^{(b)}} \left( n_{m,d} + \frac{1}{2} \right) \right) \epsilon_n^{(b_0)}(\epsilon_{n_0}^{(b_0)}, \cdot) \quad (31)$$

where we employed the energy functions,

$$E_{\text{eff},d}^{(b,p_b)} := \frac{1}{8} \left( \frac{\omega_k^{(b)} \partial \omega_k^{(b)}}{\partial b} \right)^2 \left( \frac{1}{\Sigma^2} \left( \frac{\partial \Sigma}{\partial p_b} \right)^2 - \frac{1}{\Sigma^2} \left( \frac{\partial^2 \Sigma}{\partial p_b^2} \right) \right) = -\frac{\sigma^2 \mu^4 b^2}{8 \Sigma^3} \quad (32)$$

$$E_{\text{eff},d}^{(b,p_b)} := \frac{1}{16} \left( \frac{\omega_k^{(b)} \partial \omega_k^{(b)}}{\partial b} \right)^2 \left( 2 \Sigma \frac{\partial E_G}{\partial p_b} + \frac{\partial^2 E_G}{\partial p_b^2} - \frac{1}{\Sigma} \frac{\partial^2 \Sigma}{\partial p_b^2} E_{KG,n} \right) \quad (33)$$

$$E_{\text{eff},d}^{(b,p_b)} := \frac{1}{8} \left( \frac{\omega_k^{(b)} \partial \omega_k^{(b)}}{\partial b} \right)^2 \left( -\Sigma \left( \frac{\partial E_G}{\partial p_b} \right)^2 + 2 \Sigma \left( \frac{\partial E_G}{\partial p_b} \right) \left( \frac{\partial^2 E_G}{\partial p_b^2} \right) E_{KG,n} - \frac{1}{\Sigma} \left( \frac{\partial \Sigma}{\partial p_b} \right)^2 E_{KG,n}^2 \right). \quad (34)$$
Note that these functions do not depend on the wave vector $\vec{m}$ which has been employed as a summation index in (31). They act as multiplicative functions which could be pulled out of the sums. The explicit evaluation of the energy functions shows that several terms include higher orders in the perturbation parameter $\varepsilon$. The remaining terms at second order are,

$$h_{\text{eff},2} = -\frac{3}{32} \mu_4 \sum_{d=1}^{D} e^{(b_0)}_{n_d} \langle e^{(b_0)}_{n_d}, \cdot \rangle \sum_{\vec{m} \in \Theta} \left( \frac{b^4}{\ell^3 \Sigma^3} \frac{1}{(\omega_m^{(b)})^4} \left( n_{m,d}^2 + n_{m,d} + 1 \right) + \frac{3p_2^2 b^2}{\Sigma} \frac{1}{(\omega_m^{(b)})^5} \left( n_{m,d} + \frac{1}{2} \right) \right)$$

We emphasize that the sums over all modes $\vec{m}$ in (35) converge. First, the integers $n_{m,d}$ are only non-vanishing for a finite number of modes $\vec{m}$ which solves the convergence problem for terms which enter with polynomials of $n_{m,d}$. The remaining constant contributions however benefit from the high inverse order with which, $\omega_m^{(b)} = \sqrt{\vec{m}^2 + \mu^2 b^2}$, enters.

4 Conclusion and Outlook

We have computed an effective Hamiltonian that incorporatesthe influence of the inhomo-
geneous degrees of freedom on the quantum dynamics of the homogeneous ones. We have
done this for every energy band of the Hamiltonian of the inhomogeneous degrees of freedom separately. The spectrum of these effective Hamiltonians can be computed and by rotating the corresponding (generalised) eigenvectors by the (approximate) inverse unitary operator that was used to achieve the (approximate) adiabatic decoupling of the energy bands, one obtains (approximate) eigenvectors of the original Hamiltonian that describes the interaction and mutual backreaction between the homogeneous and inhomogeneous degrees of freedom. One can then consider semiclassical states and decompose them with respect to this (approximate) generalised energy basis in order to study their quantum evolution and in particular the fate of the classical big bang singularity. We reserve this for future work.

In the final paper [15] of this series we consider General Relativity without dust coupled to an inflaton. We start from the formulation of the dynamics in terms of the canonical variables [16] which are already ideally prepared for an application of the SAPT scheme. The challenge is twofold: First, the dependence of the inhomogenous contribution to the Hamiltonian constraint on the homogeneous degrees of freedom is more complicated than for the model treated in this paper which makes the computation of the adiabatic corrections much more complicated. Second, the avoidance of the complications originating from the subset of the slow phase space where the Mukhanov-Sasaki and tensor mode mass squared functions become negative requires a more involved discussion.

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References

[1] S. Schander and T. Thiemann: “Quantum Cosmological Backreactions I: Cosmological Space Adiabatic Perturbation Theory”
[2] Viatcheslav Mukhanov. Physical foundations of cosmology. Cambridge University Press, Cambridge, 2005
[3] G. Panati, H. Spohn and S. Teufel: “Space-Adiabatic Perturbation Theory, Adv. Theor. Math. Phys. 7 (2003) 145-204.
S. Teufel: “Space Adiabatic Perturbation Theory”, Lecture Notes in Mathematics 1821, 2003.
[4] J. Neuser, S. Schander and T. Thiemann: “Quantum Cosmological Backreactions II: Purely Homogeneous Quantum Cosmology”
[5] S. Fulling. Aspects of Quantum Field Theory in Curved Spacetime. London Math. Society Student Texts, vol. 17, 1989.
[6] S. Doplicher, K. Fredenhagen, J.E. Roberts. The Quantum structure of space-time at the Planck scale and quantum fields Commun. Math. Phys. 172 (1995) 187-220 e-Print: hep-th/0303037
S. Doplicher, K. Fredenhagen, J.E. Roberts. Space-time quantization induced by classical gravity. Phys. Lett. B331 (1994) 39-44
[7] Beatriz Elizaga Navascues, Mercedes Martin-Benito, Guillermo A. Mena Marugan. Hybrid models in loop quantum cosmology Int. J. Mod. Phys. D25 (2016), 1642007. e-Print: arXiv:1608.05947
[8] Albert Messiah. Quantum Mechanics, vol. 2. Dover Publications, Dover 2017.
[9] Loop Quantum Gravity - The First 30 Years. Abhay Ashtekar, Jorge Pullin (eds.). World Scientific, Singapore, 2017.
Jorge Pullin, Rodolfo Gambini. A First Course in Loop Quantum Gravity. Oxford University Press, Oxford, 2011.
Carlo Rovelli. Quantum Gravity. Cambridge University Press, Cambridge, 2008.
Thomas Thiemann. Modern Canonical Quantum General Relativity. Cambridge University Press, Cambridge, 2007.
[10] Alexander Stottmeister, Thomas Thiemann. Coherent states, quantum gravity and the Born-Oppenheimer approximation,
I: General considerations. J. Math. Phys. 57 (2016), 063509. http://arxiv.org/abs/arXiv:1504.02169
II. Compact Lie Groups. J. Math. Phys. 57 (2016), 073501. http://arxiv.org/abs/arXiv:1504.02170
III. Applications to loop quantum gravity. J. Math. Phys. 57 (2016), 083509. http://arxiv.org/abs/arXiv:1504.02171
[11] Karel V. Kuchar, Charles G. Torre. Gaussian reference fluid and interpretation of quantum geometrodynamics. Phys. Rev. D43 (1991) 419-441.
[12] Kristina Giesel, Thomas Thiemann. Scalar Material Reference Systems and Loop Quantum Gravity. Class. Quant. Grav. 32 (2015), 135015. arXiv:1206.3807
[13] K. Giesel, S. Hofmann, T. Thiemann, O. Winkler. Manifestly Gauge-Invariant General Relativistic Perturbation Theory.
I. Foundations Class. Quant. Grav. 27 (2010) 055005. e-Print: arXiv:0711.0115
II. FRW background and first order. Class. Quant. Grav. 27 (2010) 055006. e-Print: arXiv:0711.0117
[14] J. David Brown, Karel V. Kuchar. Dust as a standard of space and time in canonical quantum gravity. Phys. Rev. D51 (1995) 5600-5629. e-Print: gr-qc/9409001
[15] S. Schander, T. Thiemann. Quantum Cosmological Back Reactions IV: Constrained quantum cosmological perturbation theory
[16] Laura Castello Gomar, Mercedes Martin-Benito, Guillermo A. Mena Marugan. Gauge-Invariant Perturbations in Hybrid Quantum Cosmology JCAP 1506 (2015), 045. e-Print: arXiv:1503.03907
Laura Castello Gomar, Mercedes Martin-Benito, Guillermo A. Mena Marugan. Quantum corrections to the Mukhanov-Sasaki equations. Phys. Rev. D93 (2016), 104025. e-Print: arXiv:1603.08448

[17] Martin Bojowald. Loop quantum cosmology Living Rev. Rel. 11 (2008) 4
Mathematical structure of loop quantum cosmology Abhay Ashtekar, Martin Bojowald, Jerzy Lewandowski. Adv. Theor. Math. Phys. 7 (2003), 233-268. gr-qc/0304074.
Abhay Ashtekar, Tomasz Pawlowski, Parampreet Singh. Quantum Nature of the Big Bang: Improved dynamics. Phys. Rev. D74 (2006) 084003. e-Print: gr-qc/0607039

[18] Thomas Thiemann. Properties of a smooth, dense, invariant domain for singular potential Schrödinger operators. In preparation.