Quantum cosmological backreactions. III. Deparametrized quantum cosmological perturbation theory

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(Received 2 July 2021; accepted 28 March 2022; published 16 May 2022)

This is the third paper in a series of four in which we incorporate backreaction among the homogeneous as well as between the homogeneous and inhomogeneous degrees of freedom in quantum cosmological perturbation theory using space adiabatic methods. Here, we consider a gauge-fixed version of cosmological perturbation theory which uses Gaussian dust as a material reference system. The observable matter content is a real-valued scalar field. We explore the sector of that theory which is purely homogeneous and isotropic with respect to the geometry degrees of freedom but which contains inhomogeneous perturbations up to second order of the scalar field. We explore the quantum field theoretical challenges of the space adiabatic framework in a cosmological model of the early universe which is technically still relatively simple. We compute the quantum backreaction effects from the inhomogeneous matter modes on the homogeneous geometry up to second order in the adiabatic parameter. It turns out that these contributions are not negligible.

DOI: 10.1103/PhysRevD.105.106011

I. INTRODUCTION

The considerable amount of cosmological measurement data, collected especially within the last few years, allows one to study ever more distant regions of the Universe [1–3]. Although many of these measurements provide a mostly coherent picture of the Universe's history, numerous questions remain open, e.g., the nature of dark matter and dark energy [4,5] as well as the present discrepancies between different measurement methods of the Hubble parameter [6,7] (see also [8,9] for a different assessment of the data).

One possibility to extend the cosmological paradigm in accordance with the successful Standard Model of particle physics and general relativity is to combine the two into a theory of quantum gravity. In this work, we take this possibility as a premise to investigate a cosmological theory for the earliest moments of the Universe. In particular, the study aims at understanding the interactions between the different components in a purely quantum mechanical universe which consists of the purely homogeneous and isotropic degrees of freedom of standard cosmology and perturbations of a scalar matter field thereon. With this, we build on the two previous works in this series of four papers [10,11] which focus on the technical realization of our approach and the investigation of a simplified cosmological model. In the fourth paper [12], we consider a cosmological perturbation theory with gauge-invariant perturbations of gravity and scalar matter but, in contrast to the present work, we do not introduce additional dust fields to deparametrize the system.

The basic idea of our approach relies on the Born-Oppenheimer theory for molecules for coupled quantum systems that exhibit very different rates of change among their constituents [13]. The scheme allows one to establish effective quantum equations of motion for the so-called "slow" degrees of freedom which take the backreactions of the so-called "fast" degrees of freedom into account. In our cosmological setting, the homogeneous and isotropic subsector of the model identifies with the heavy degrees of freedom while the perturbations play the role of the light variables. That this assumption is indeed physically reasonable results from the identification of the homogeneous variables with a "heavy" and slow center of mass mode as we argue in the first paper [10]. There, we further assert that the Born-Oppenheimer theory has only a very limited range of validity and that its approximations fail for interesting dynamical time periods.

Fortunately, it is possible to resort to a more refined approximation scheme which is known as space adiabatic perturbation theory (SAPT) [14,15]. The Born-Oppenheimer approximation is its restriction to zeroth perturbative order, and also applies to a broader range of systems [10].

Since SAPT was initially developed for systems with a finite number of degrees of freedom, it is first necessary to extend the formalism to systems with an infinite number of

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degrees of freedom. This has been first considered in [16–18], and subsequently in our first paper [10], and we will come to the resulting challenges in the next section. Due to its very structure, this extension will allow us to use the framework of quantum field theory on curved spacetimes (QFT on CST) [19], while accounting for the quantum nature of the homogeneous degrees of freedom.

In this paper, we consider general relativity coupled to a real Klein-Gordon matter field and to Gaussian dust [20]. The dust fields serve to deparametrize the theory [21] such that the geometric degrees of freedom along with the scalar field become (Dirac) observables. Consequently, the system has a true conservative Hamiltonian which for Gaussian dust reveals to be particularly simple: it solely consists of the gravitational and scalar matter contributions to the Hamilton constraint integrated over space. This classical Hamilton function can then be decomposed into a homogeneous and a linearly perturbed part (up to second order) in accordance with standard classical perturbation theory. In Ref. [22,23], this has been investigated in the same fashion in all detail for a different material reference system [24].

For the illustrative purpose of this paper, we discard the inhomogeneous geometry degrees of freedom and focus on the inhomogeneous scalar matter fields as we aim at illustrating the space adiabatic formalism in a cosmological, quantum field theoretical context which is as simple as possible. The study generalizes directly to the model with inhomogeneous geometry modes [12]. In both cases, the application of the space adiabatic scheme to a quantum field model proceeds in the same lines as for the purely homogeneous quantum mechanical model in [11] but with two important differences.

First, the scheme requires one to perform a transformation which is canonical up to second order in the perturbations. This has the crucial purpose of obtaining a new set of variables in terms of which the background dependent Fock representations of the scalar field modes employ all the same Hilbert space (see [10] for more details). The transformations employed here, as well as in [25,26] in a different context, restore the unitary equivalence of the QFT Hilbert spaces and allow one to employ SAPT.

The second step for the application of SAPT consists in a canonical transformation exlusively for the homogeneous degrees of freedom with the aim of avoiding tachyonic quantum fields. Indeed, the preceding transformations can cause the occurrence of indefinite mass squared values for the quantum fields [10]. We emphasize, however, that the occurrence of such tachyonic instabilities is *not due to the SAPT scheme itself*, but already occurs in standard gauge-invariant cosmological perturbations theory, e.g., when using Mukhanov-Sasaki variables [27]. While cases of indefinite mass squared functions appear frequently in the literature (see for example [28]), the introduction of such tachyonic fields raises some important questions, e.g., about the effects of such an instability, and the question of renormalizability and Lorentz invariance [29,30]. Most important, the issue here is the following: If one treats the background variables as external parameters, one can restrict them by hand to a region of the homogeneous phase space where the effective mass squared is positive. However, when taking the full backreaction into account, the homogeneous quantum phase can no longer be restricted by hand. One can also not use some kind of semiclassical argument when performing the spectral analysis of the fully backreacting total Hamiltonian. Hence, we pursue the strategy to avoid such instabilities (and all subsequent problems) and present an approach for how to obtain a positive definite mass square for the matter scalar field by means of canonical transformations for the homogeneous sector.

After these subtleties have been dealt with, we proceed as in [11] and compute the second order space adiabatic corrections to the dynamics of the homogeneous *quantum* degrees of freedom *including* the backreactions from the inhomogeneous quantum scalar field.

We emphasize that there are two different perturbation schemes: The cosmological perturbation theory and the space adiabatic perturbation scheme. The perturbative adiabatic corrections due to SAPT turn out to be highly nontrivial and to be sensitive to the Fock representation chosen in the inhomogeneous sector.

In hitherto existing approaches to quantum cosmology, such as loop quantum cosmology (LQC) [31–33], this specific kind of adiabatic backreaction has not been investigated in detail so far. We emphasize, however, that the hybrid LQC approach [34] already includes a different kind of backreaction by correcting the homogeneous variables by perturbative contributions [25] (and which is also taken into account in this series of papers). With this work, we hope to make a decisive step toward a complete implementation of the interactions and backreactions in perturbative quantum cosmology.

The architecture of this paper is as follows. In Sec. II, we briefly introduce the model and prepare it for the application of SAPT by performing the aforementioned field truncations and canonical transformations. In Sec. III, we apply the space adiabatic framework to the model. Our result here shows that 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 [35]. In Sec. IV, we summarize our findings and conclude.

II. COSMOLOGICAL PERTURBATIONS WITH DUST

A. The Hamiltonian

We consider a four-dimensional globally hyperbolic spacetime manifold $\mathcal{M}$ which foliates into spatial hypersurfaces $\mathcal{B}$ according to $\mathcal{M} \cong \mathbb{R} \times \mathcal{B}$. We assume $\mathcal{B}$ to be a

three-dimensional compact and flat manifold with volume l^3. Since any compact and flat manifold can be reduced to a torus of the corresponding dimension, we can assume without loss of generality that $\mathcal{B} = \mathbb{T}^3$. We identify points and coordinates and use lowercase letters "x" for points and coordinates on $\mathcal{B}$. Our model consists, on the one hand, of the gravitational degrees of freedom, i.e., the metric g and its covariant derivative, based on Einstein's general relativity with the Einstein-Hilbert action S_{EH} [36]. We restrict the gravitational degrees of freedom to its purely spatially homogeneous and isotropic contribution such that the only relevant degrees of freedom are the time-dependent scale factor a, its velocity $\dot{a}$, and the lapse function N. On the other hand, we include a real-valued and timelike scalar dust field u with energy density ρ which is homogeneous and isotropic as well [21,24]. The dust field deparametrizes the model and transforms the Hamilton constraint into a physical Hamilton function for the gravitational and the additional matter degrees of freedom. For the matter sector of the system, we choose a real-valued scalar field Φ of Klein-Gordon type with mass $m \in \mathbb{R}^+$ and coupling constant $\lambda \in \mathbb{R}^+$.

Following the idea of Halliwell and Hawking [37], we develop the Klein-Gordon field action S_{KG} in the perturbative fields up to second order. This, together with the homogeneous contributions from gravity and the dust field, yields the total action $S = S_{\mathrm{hom}} + S_{\mathrm{pert}}$ with

$$S_{\mathrm{hom}}[a,N,u] = l^3 \int_{\mathbb{R}} \mathrm{d}t\, N\left(-\frac{3a}{\kappa}\left(\frac{\dot{a}}{N}\right)^2 - \frac{\Lambda}{\kappa}a^3 + a^3\frac{\rho}{2}\left(\left(\frac{\dot{u}}{N}\right)^2 - 1\right)\right), \tag{1}$$

$$S_{\mathrm{pert}}[a,N,\Phi] = \frac{1}{2\lambda}\int_{\mathbb{R}\times\mathcal{B}} \mathrm{d}t\,\mathrm{d}x\,\sqrt{h^0}Na^3\left(\left(\frac{\dot{\Phi}}{N}\right)^2 - \frac{1}{a^2}\Phi(-\Delta + a^2m^2)\Phi\right). \tag{2}$$

$\kappa = 8\pi G$ denotes the gravitational coupling constant and $\Lambda \in \mathbb{R}^+$ is an additional cosmological constant. $\sqrt{h^0}$ is the volume element of the spatial manifold $\mathcal{B}$ which in the case of a flat torus is simply 1 since the spatial metric reduces to the standard Euclidean metric restricted to a corresponding domain. Δ is the Laplace-Beltrami operator on $\mathbb{T}^3$ and t is cosmic time.

To conduct the necessary Hamiltonian analysis for the space adiabatic scheme, we perform a Legendre transformation with the Lagrange function and density defined by $S = \int \mathrm{d}t L = \int \mathrm{d}t\,\mathrm{d}x\,\mathcal{L}$, and introduce the conjugate momenta

$$P_a := \frac{\partial L}{\partial \dot{a}} = -6\frac{l^3}{\kappa N}a\dot{a}, \qquad \Pi := \frac{\partial \mathcal{L}}{\partial \dot{\Phi}} = \frac{a^3}{\lambda N}\dot{\Phi}. \tag{3}$$

The constraint analysis reveals that the lapse function is a mere Lagrange multiplier such that we can set $N \equiv 1$ without loss of generality. Due to the dust field, the linear constraints can be solved immediately by using a reduced phase space scheme. As a consequence, the system has a physical Hamilton function $H = H_{\mathrm{hom}} + H_{\mathrm{pert}}$ with

$$H = -\frac{\kappa}{12l^3}\frac{P_a^2}{a} + \frac{l^3}{\kappa}\Lambda a^3 + \frac{\lambda}{2a^3} \times \int_{\mathbb{T}^3} \mathrm{d}x\left(\Pi^2 + \frac{a^4}{\lambda^2}\Phi(-\Delta + a^2m^2)\Phi\right). \tag{4}$$

The canonical structure of the system is encoded in the Poisson bracket relations

$$\{a, P_a\} = 1,$$
$$\{\Phi(f_1), \Pi(f_2)\} = \int_{\mathbb{T}^3} \mathrm{d}x\, f_1(x)f_2(x) =: \langle f_1, f_2\rangle, \tag{5}$$

where $f_1, f_2 \in C_0^\infty(\mathbb{T}^3)$ are test functions on the torus and all other Poisson brackets vanish. In order to make the space adiabatic scheme work at the technical level, it is necessary to rescale the momentum of the slow subsystem by a small parameter ε. In the given case, the gravitational coupling constant κ or more precisely the dimensionless combination $\kappa/\lambda := \varepsilon^2$ is a suitable choice.

As explained in the companion paper [10], it is reasonable to identify the homogeneous and isotropic degrees of freedom with a heavy center of mass mode such that the homogeneous geometry plays the role of the slow subsystem here. Let us define a rescaled momentum associated with the scale factor by $p_a := \varepsilon P_a$. To simplify notation, we also define a rescaled cosmological constant which we assume still to be very small, namely $\tilde{\Lambda} := \Lambda/\varepsilon^2$, and we set λ to unity without loss of generality. The homogeneous contribution to the Hamilton operator has consequently the form

$$H_{\mathrm{hom}} = -\frac{1}{12l^3}\frac{p_a^2}{a} + l^3\tilde{\Lambda}a^3. \tag{6}$$

The Poisson bracket of the gravitational subsystem transforms into $\{a, p_a\} = \varepsilon$. It turns out that this rescaling makes the perturbative space adiabatic scheme work out properly. Before applying the scheme, we need to assure that the QFT associated with the fields (Φ, Π) allow for unitarily equivalent Hilbert space representations for different background configurations (a, p_a). As it turns out, this requires an additional "almost" canonical transformation for the whole system.

B. Almost canonical transformation

The inhomogeneous part of the Hamilton function in Eq. (4) depends on the scale factor and contains, in particular, an a-dependent effective frequency operator

$$\omega(a) := \sqrt{-a^4\Delta + m^2 a^6}. \tag{7}$$

It turns out that the a-dependence of the Laplace term in $\omega(a)$ prevents the QFT of (Φ, Π) from having unitarily equivalent representations for different values of the scale factor [10]. To address this problem, we perform a transformation of variables for the totality of the system which is canonical up to second order in the perturbative fields. Such transformations have been widely used in the hybrid LQC community for the same purpose, and we refer exemplarily to [25] where a very similar model was treated (leading to the same transformations up to the choice of variables). In order to ensure that the transformation is almost canonical, we first consider the symplectic one-form Θ which is a function on the tangent space of the total phase space having values in $\mathbb{R}$.

In coordinate representation, in which $\mathrm{d}a$ and $\mathrm{d}\Phi$ represent the standard one-forms for the homogeneous and the inhomogeneous phase spaces, respectively, we have that Θ is given by

$$\begin{aligned}\Theta &= P_a \mathrm{d}a + \int_{\mathbb{T}^3} \mathrm{d}x\, \Pi(x)\mathrm{d}\Phi(x)\\ &= \frac{1}{\varepsilon} p_a \mathrm{d}a + \int_{\mathbb{T}^3} \mathrm{d}x\, \Pi(x)\mathrm{d}\Phi(x).\end{aligned} \tag{8}$$

In order to eliminate the a-dependence of the Laplace term in the Hamiltonian (4), it seems reasonable to rescale the field variable Φ such that a factors out; see [38] and references therein where this idea has also been used. Anticipating that this transformation alone is not (almost) canonical, we define a more general transformation for the field variables by

$$\begin{aligned}&\tilde{\Phi} := a \cdot \Phi, \qquad \tilde{\Pi} := \frac{\Pi}{a} + a\eta(a, p_a)\cdot\Phi \Rightarrow \Phi = \frac{\tilde{\Phi}}{a},\\ &\Pi = a\cdot(\tilde{\Pi} - \eta(a, p_a)\cdot\tilde{\Phi}),\end{aligned} \tag{9}$$

where we introduced a real-valued function $\eta(a, p_a)$ on the slow phase space which we are going to determine by the requirement of obtaining a well-defined QFT at the end. Besides, the following abbreviations will prove to be useful:

$$A := \int_{\mathbb{T}^3} \mathrm{d}x\, \Phi(x)^2 = \frac{1}{a^2}\int_{\mathbb{T}^3} \mathrm{d}x\, \tilde{\Phi}(x)^2 =: \frac{\tilde{A}}{a^2}, \tag{10}$$

$$\begin{aligned}B &:= \int_{\mathbb{T}^3} \mathrm{d}x\, \Pi(x)\Phi(x)\\ &= \int_{\mathbb{T}^3} \mathrm{d}x\, \tilde{\Pi}(x)\tilde{\Phi}(x) - \eta(a, p_a)\tilde{A} =: \tilde{B} - \eta\cdot\tilde{A}.\end{aligned} \tag{11}$$

We insert the transformations (9) into the symplectic potential Θ and use the definitions, Eqs. (10) and (11). The product rule for the differential one-form which we apply on $\tilde{\Phi}/a$ and omitting total differentials then yields

$$\Theta = \left(\frac{1}{\varepsilon}p_a - \frac{1}{a}\tilde{B} + \frac{\eta}{a}\tilde{A}\right)\mathrm{d}a + \int_{\mathbb{T}^3} \mathrm{d}x\, \tilde{\Pi}\mathrm{d}\tilde{\Phi} + \frac{\tilde{A}}{2}\mathrm{d}\eta. \tag{12}$$

Since η depends solely on a and p_a, we can write $\mathrm{d}\eta = \eta_{,a}\,\mathrm{d}a + \eta_{,p_a}\,\mathrm{d}p_a$, where the comma corresponds to the derivative with respect to the given variable. The term proportional to $\mathrm{d}a$ fits nicely into the first bracket in Eq. (12). For the second term, we use that total differentials vanish and by cutting the theory after second order in the scalar field variables, the symplectic potential has the form

$$\begin{aligned}\Theta = &\left(\frac{1}{\varepsilon}p_a - \frac{1}{a}\tilde{B} + \frac{\eta}{a}\tilde{A} + \frac{1}{2}\eta_{,a}\tilde{A}\right)\mathrm{d}\left(a - \frac{1}{2}\varepsilon\eta_{,p_a}\tilde{A}\right)\\ &+ \int_{\mathcal{B}} \mathrm{d}x\, \tilde{\Pi}\mathrm{d}\tilde{\Phi}.\end{aligned} \tag{13}$$

This structure gives rise to the definition of new variables in the homogeneous sector,

$$\begin{aligned}&\tilde{p}_a := p_a + \varepsilon\left(-\frac{1}{a}\tilde{B} + \frac{\eta}{a}\tilde{A} + \frac{1}{2}\eta_{,a}\tilde{A}\right),\\ &\tilde{a} := a - \frac{1}{2}\varepsilon\eta_{,p_a}\tilde{A}.\end{aligned} \tag{14}$$

Expressed with these new dashed variables for both the homogeneous and the inhomogeneous sectors, the symplectic potential regains its original standard form. It remains to determine the function $\eta(a, p_a)$ and to verify whether the Hamilton function transforms into a well-defined function with respect to the new variables. In order to express the Hamilton function in terms of them, the conversion rules (14) need to be inverted. It proves to be beneficial to directly employ an explicit choice for the function η. An educated guess is

$$\eta(a, p_a) = -\frac{\varepsilon}{6l^3}\frac{p_a}{a}. \tag{15}$$

Its derivatives with respect to p_a serve for determining a as a function of the dashed variables [cf. (14)]. Multiplying the equation for $\tilde{a}$ in (14) by a, using an algebraic solution formula for quadratic equations, and cutting again after second order in the perturbative fields give as a solution for a the second relation in (16). To determine p_a as a function of $\tilde{a}$ and $\tilde{p}_a$ we insert the solution for $a(\tilde{a}, \tilde{p}_a)$ into the first relation in (14) and Taylor expand the function up to second order in the perturbation fields. This yields

$$p_a = \tilde{p}_a + \varepsilon\frac{1}{\tilde{a}}\tilde{B} + \frac{\varepsilon^2}{12l^3}\frac{\tilde{p}_a}{\tilde{a}}\tilde{A}, \qquad a = \tilde{a} - \frac{\varepsilon^2}{12l^3\tilde{a}}\tilde{A}. \tag{16}$$

In the first step, we compute the homogeneous part of the Hamilton function (6) in terms of the dashed variables and

eventually compare it with the perturbative part. We use the assignment rules (16) and Taylor expand again up to second order in the perturbation fields. For the homogeneous part, now including also second order contributions, we get the following result:

$$\tilde{H}_{\mathrm{hom}} = -\frac{1}{12l^3}\frac{\tilde{p}_a^2}{\tilde{a}} + l^3\tilde{\Lambda}\,\tilde{a}^3 - \frac{\varepsilon}{6l^3}\frac{\tilde{p}_a}{\tilde{a}^2}\tilde{B} - \frac{\varepsilon^2}{48l^6}\frac{\tilde{p}_a^2}{\tilde{a}^3}\tilde{A} - \frac{\Lambda}{4}\tilde{a}\,\tilde{A}\,. \tag{17}$$

The first two terms agree with the original homogeneous Hamilton function but with dashed variables. The additional terms are second order in the fields and arise because of the transformations. In particular, the $\tilde{B}$-term introduces difficulties because its quantization is not a well-defined operator on Fock space. Fortunately, the definition of the function $\eta(a, p_a)$ was aimed exactly at canceling the term with the transformed, inhomogeneous Hamilton function. Indeed, the latter reads in terms of the dashed variables by omitting any contributions of third order and higher in the fields,

$$\tilde{H}_{\mathrm{pert}} = \frac{1}{2\tilde{a}}\int_{\mathbb{T}^3} \mathrm{d}x\,(\tilde{\Pi}^2 + \tilde{\Phi}(-\Delta + \tilde{a}^2m^2)\tilde{\Phi}) + \frac{\varepsilon}{6l^3}\frac{\tilde{p}_a}{\tilde{a}^2}\tilde{B} + \frac{\varepsilon^2}{72l^6}\frac{\tilde{p}_a^2}{\tilde{a}^3}\tilde{A}. \tag{18}$$

We observe that the a-dependence of the Laplace term has indeed vanished and a global factor $\tilde{a}^{-1}$ has appeared for the classical Klein-Gordon Hamilton function. Besides, the transformation yields new terms which indeed cancel the anomalous contribution of the dashed homogeneous Hamilton function (17). In total, the Hamiltonian $\tilde{H} = \tilde{H}_{\mathrm{hom}} + \tilde{H}_{\mathrm{pert}}$ gives rise to two supplementary, independent contributions that depend on $\tilde{A}$. Recalling the definition of $\tilde{A} = \int \mathrm{d}x\,\Phi^2$ in (10), they yield additional contributions to an effective mass function $M(\tilde{a}, \tilde{p}_a)$. In particular, this gives

$$\tilde{H} = -\frac{1}{12l^3}\frac{\tilde{p}_a^2}{\tilde{a}} + l^3\tilde{\Lambda}\,\tilde{a}^3 + \frac{1}{2\tilde{a}}\int_{\mathbb{T}^3} \mathrm{d}x\,(\tilde{\Pi}^2 + \tilde{\Phi}(-\Delta + \tilde{a}^2M(\tilde{a}, \tilde{p}_a)^2)\tilde{\Phi}), \tag{19}$$

$$\text{with}\quad M(\tilde{a}, \tilde{p}_a)^2 = \left(m^2 - \frac{\Lambda}{2}\right)\tilde{a}^2 - \frac{\varepsilon^2}{72l^6}\frac{\tilde{p}_a^2}{\tilde{a}^2}. \tag{20}$$

The Laplace term in the perturbative part of this Hamilton function no longer depends on the scale factor. After a quantization of the fields, the Fock representations are consequently unitarily equivalent for different background configurations. This allows one to finally apply the space adiabatic perturbation scheme. However, we face the problem that the effective mass square function (20) of the correspondent field theory is indefinite, thus leading to tachyonic instabilities for certain regions in the slow phase space Γ_{hom}. We refer to the companion paper [10], where we present several strategies for how to deal with this issue. Here, we perform an additional canonical transformation (in its restricted domain of definition) with respect to the homogeneous variables only such that the effective mass squared becomes positive definite in terms of these variables. Therefore, let us define a set of constant parameters which help to define such new variables,

$$\mu^2 := m^2 - \frac{\Lambda}{2}, \qquad \tau^2 := \frac{\varepsilon^2}{72l^6}, \qquad \sigma^2 := \frac{\tau^2}{\mu^2}. \tag{21}$$

We assume the constant $m^2 - (\Lambda/2)$ to be positive such that σ is in the reals. In terms of these parameters, the effective mass value becomes $M^2 =: \mu^2\tilde{a}^2 - \tau^2(\tilde{p}_a^2/\tilde{a}^2)$. We then choose a new canonical pair (b, p_b) according to the transformation rules

$$\tilde{a} =: \sqrt{b^2 + \sigma^2\frac{p_b^2}{b^2}} =: \beta(b, p_b), \qquad \tilde{p}_a =: \tilde{a}\,\frac{p_b}{b}. \tag{22}$$

The effective mass square function is then simply given by $M^2 = \mu^2b^2$ which is positive for any $b \in \mathbb{R}$. By this choice, we implicitly limit the original phase space in terms of $(\tilde{a}, \tilde{p}_a)$ to a restricted domain. Note that this transformation is similar to the procedure in quantum cosmology where one trades (a, p_a) for (e, p_e) with $a^2 = e^2$ and $a \geq 0$ but $e \in \mathbb{R}$ is the homogeneous triad. This choice corresponds to a working proposal in order to circumvent the tachyonic instabilities.

After all, the starting point for SAPT is then the Hamilton function in terms of the new variables,

$$H = -\frac{1}{12l^3}\beta\frac{p_b^2}{b^2} + l^3\tilde{\Lambda}\beta^3 + \frac{1}{2\beta} \times \int_{\mathbb{T}^3} \mathrm{d}x\,(\tilde{\Pi}^2 + \tilde{\Phi}(-\Delta + \mu^2b^2)\tilde{\Phi}). \tag{23}$$

Now, SAPT necessitates a Hamilton operator $\hat{\boldsymbol{H}}$ whose classical counterpart is H and which is an operator on (a dense domain of) the total Hilbert space $\mathcal{H}$ of the system. Here, we consider the quantization of H with respect to both, the homogeneous and the inhomogeneous subsector to obtain the operator $\hat{\boldsymbol{H}}$.

We start by considering the quantization of the homogeneous degrees of freedom (b, p_b), and we employ the standard Schrödinger representation. We label quantum operators by hats; for example we write $\hat{b}$ and $\hat{p}_b$ for the canonical quantum operators. We recall that b and p_b arose from the rescaled variables $\tilde{a}$ and $\tilde{p}_a$ such that the canonical commutation relation is given by $[\hat{b}, \hat{p}_b] = i\varepsilon\hat{1}_{\mathrm{hom}}$. Regarding the ordering of noncommuting operators, we employ the symmetric Weyl quantization procedure for the

homogeneous sector. In general, we denote the Weyl quantization of a function $f \in C^\infty(\Gamma_{\mathrm{hom}}, \mathbb{R})$ by $\hat{\mathcal{W}}(f)$. The Hilbert space of the homogeneous sector is supposed to be the space of square integrable functions $L^2(\mathbb{R}, \mathrm{d}b)$ with the standard measure on $\mathbb{R}$.

For the inhomogeneous sector, we choose a standard Fock representation on $\mathbb{T}^3$. Therefore, consider the one-particle Hilbert space $\mathcal{H}_{\mathbb{T}^3} = L^2(\mathbb{T}^3, \mathrm{d}x)$ on $\mathbb{T}^3$. Since the effective frequency operator $\omega(b) \coloneqq \sqrt{-\Delta + \mu^2 b^2}$ depends on the homogeneous variable b, any Fock representation for a different effective mass value $\mu^2 b^2$ could fail to be unitarily equivalent. However, the almost canonical transformations from above guarantee that all these Fock representations are mutually unitarily equivalent, at least up to second order in the field perturbations. Therefore, one can choose any of the symmetric Fock representations $\pi_b : \mathcal{A}_Q \to \mathcal{L}(\mathcal{F}_{\mathrm{s}})$ for some fixed $b \in \mathbb{R}$ that map the field Weyl algebra $\mathcal{A}_Q$ into the space of linear operators on the Fock space $\mathcal{F}_{\mathrm{s}}$. We label operators acting on $\mathcal{F}_{\mathrm{s}}(\mathcal{H}_{\mathbb{T}^3})$ with bold letters such that the basic field operators are $\boldsymbol{\Phi}(f_1)$ and $\boldsymbol{\Pi}(f_2)$ for some smooth test functions f_1 and f_2 on $\mathbb{T}^3$. The Fock space $\mathcal{F}_{\mathrm{s}}$ consists of sequences $\{\psi_{(n)}\}_{n\geq 0}$ of totally symmetric functions with n variables x_i. The canonical commutation relations are given by

$$[\boldsymbol{\Phi}(f_1), \boldsymbol{\Pi}(f_2)] = i\langle f_2, f_2\rangle \mathbf{1}_{\mathrm{pert}}. \tag{24}$$

It is also admissible to identify the field operators with operator-valued distributions $\boldsymbol{\Phi}(x)$ and $\boldsymbol{\Pi}(x)$ such that $\boldsymbol{\Phi}(f) = \int \mathrm{d}x\, \boldsymbol{\Phi}(x) f(x)$ and similarly for its conjugate momentum $\boldsymbol{\Pi}$. Finally, we aim at connecting the quantum theories of the homogeneous and the inhomogeneous subsectors. We therefore define the total Hilbert space to be the topological tensor product $\mathcal{H} \coloneqq \mathcal{H}_{\mathrm{hom}} \otimes \mathcal{H}_{\mathrm{pert}} = L^2(\mathbb{R}, \mathrm{d}b) \otimes \mathcal{F}_{\mathrm{s}}$. With these prerequisites, the Hamilton operator $\hat{\boldsymbol{H}}$ acting on a dense subset $\mathcal{D} \subset \mathcal{H}$ of the total Hilbert space has the form

$$\begin{aligned}\hat{\boldsymbol{H}} = {} & \hat{\mathcal{W}}\left(-\frac{1}{12l^3}\beta\frac{p_b^2}{b^2} + l^3\tilde{\Lambda}\beta^3\right) \otimes \mathbf{1}_{\mathrm{hom}} \\ & + \frac{1}{2}\hat{\mathcal{W}}(\beta^{-1}) \otimes \int_{\mathbb{T}^3} \mathrm{d}x\, \boldsymbol{\Pi}(x)^2 \\ & + \frac{1}{2}\hat{\mathcal{W}}(\beta^{-1}) \otimes \int_{\mathbb{T}^3} \mathrm{d}x\, \boldsymbol{\Phi}(x)(-\Delta\boldsymbol{\Phi})(x) \\ & + \frac{\mu^2}{2}\hat{\mathcal{W}}(\beta^{-1}b^2) \otimes \int_{\mathbb{T}^3} \mathrm{d}x\, \boldsymbol{\Phi}(x)^2. \end{aligned} \tag{25}$$

III. APPLICATION OF SPACE ADIABATIC PERTURBATION THEORY

A. Conditions for space adiabatic perturbation theory

SAPT according to Panati, Spohn, and Teufel [14,15] applies to a variety of systems but it must be ensured that the conditions listed below are met. We present and directly discuss these requirements for our model.

(C1) *The state space* of the system decomposes as

$$\mathcal{H} = L^2(\mathbb{R}) \otimes \mathcal{H}_{\mathrm{f}} = L^2(\mathbb{R}, \mathcal{H}_{\mathrm{f}}), \tag{26}$$

where $L^2(\mathbb{R})$ is the state space of the slow subsystem and $\mathcal{H}_{\mathrm{f}}$ must be a separable Hilbert space associated with the fast subsystem.

Our cosmological system satisfies this first condition thanks to the almost canonical transformation up to second order in the perturbations. The transformations guarantee that the fast Hilbert spaces, i.e., the Fock spaces $\mathcal{F}_{\mathrm{s}}(b, \mathcal{H}_{\mathbb{T}^3})$ are all unitarily equivalent for different $b \in \mathbb{R}$ for the truncated system such that we can simply write $\mathcal{F}_{\mathrm{s}}(\mathcal{H}_{\mathbb{T}^3})$. The total Hilbert space is thus given by $\mathcal{H} = L^2(\mathbb{R}, \mathrm{d}b) \otimes \mathcal{F}_{\mathrm{s}}(\mathcal{H}_{\mathbb{T}^3})$. Besides, $\mathcal{F}_{\mathrm{s}}(\mathcal{H}_{\mathbb{T}^3})$ is separable because the one-particle Hilbert space is given by $\mathcal{H}_{\mathbb{T}^3} = L^2(\mathbb{T}^3, \mathrm{d}x)$. The next condition is the following:

(C2) *The Hamilton operator* $\hat{\boldsymbol{H}}$ is the Weyl quantization of a function on the slow phase space $\boldsymbol{H}(b, p_b)$ which belongs to a so-called "symbol class" of functions $S^m_\rho(\Gamma_{\mathrm{s}}, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ with values in the bounded operators $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$ on the fast Hilbert space. The Weyl quantization refers to the slow subsystem and the function $\boldsymbol{H}(b, p_b)$ has values in the space of bounded self-adjoint operators on $\mathcal{H}_{\mathrm{f}}$.

For condition (C2), let us consider the formal quantization of the Hamilton function in (23) with respect to the inhomogeneous field perturbations only or, in other terms, the Wigner-Weyl transform of the Hamilton operator, Eq. (25), with respect to the slow subsector. This gives rise to an operator-valued function on the slow phase space, namely

$$\begin{aligned}\boldsymbol{H}(b, p_b) = {} & \left(-\frac{1}{12l^3}\beta\frac{p_b^2}{b^2} + l^3\tilde{\Lambda}\beta^3\right)\mathbf{1}_{\mathrm{pert}} \\ & + \frac{1}{2\beta}\int_{\mathbb{T}^3} \mathrm{d}x\, (\tilde{\boldsymbol{\Pi}}^2 + \tilde{\boldsymbol{\Phi}}(-\Delta + \mu^2 b^2)\tilde{\boldsymbol{\Phi}}). \end{aligned} \tag{27}$$

The Weyl quantization with respect to the homogeneous sector of this symbol function coincides with $\hat{\boldsymbol{H}}$ in (25) such that $\boldsymbol{H}(b, p_b)$ corresponds indeed to the symbol function alluded to in (C2).

It is useful to perform a transformation to annihilation and creation operators which we denote by $\boldsymbol{a}(b, f)$ and $\boldsymbol{a}^*(b, f)$ for some one-particle state $f \in L^2(\mathbb{T}^3, \mathrm{d}x)$ and for some fixed $b \in \mathbb{R}$. They shall act in the standard way. $\boldsymbol{a}(b, f)$ has the standard form with respect to the field operators and the one-particle frequency operator $\omega(b) = \sqrt{-\Delta + \mu^2 b^2}$,

$$\boldsymbol{a}(b, f) \coloneqq \frac{1}{\sqrt{2}}\pi_b[(\sqrt{\omega(b)}\tilde{\boldsymbol{\Phi}})(f) - i(\sqrt{\omega(b)}^{-1}\tilde{\boldsymbol{\Pi}})(f)]. \tag{28}$$

Together with $\boldsymbol{a}^*(b,f)$, they satisfy the canonical commutation relation, $[\boldsymbol{a}(b,f_1),\boldsymbol{a}^*(b,f_2)] = \mathbf{1}_{\mathrm{pert}}\langle f_1,f_2\rangle$. As we clarify in the course of discussing the next condition $(\mathrm{C3})_\gamma$, SAPT requires one to select a subspace of the perturbative Fock space $\mathcal{F}_\mathrm{s}$. It is thus reasonable to select an orthonormal basis of the Hilbert space $\mathcal{H}_{\mathbb{T}^3}$ to characterize the Fock states by means of their mode number.

An orthonormal eigenbasis of $\mathbb{T}^3$ is provided by the set of exponentials, $\{f_k(x) \coloneqq l^{-\frac{3}{2}}\exp(ikx)\}$ with $k \in \Sigma = \frac{2\pi}{l}\mathbb{Z}^3$. We denote the annihilation and creation operators with respect to the f_k's by $\boldsymbol{a}_k(b)$ and $\boldsymbol{a}_k^*(b)$. The correspondent commutation relation is given by $[\boldsymbol{a}_k(b),\boldsymbol{a}_{k'}^*(b)] = \delta_{k,k'}\mathbf{1}_{\mathrm{pert}}$, where δ is the Kronecker delta. The basis functions f_k diagonalize the Laplace operator, and the respective eigenvalues are given by $-\Delta f_k =: k^2 f_k$. The eigenvalues of the frequency operator $\omega(b)$ are given by $\omega_k(b) \coloneqq \sqrt{k^2+\mu^2 b^2}$. The resulting normal-ordered Hamiltonian reads

$$\boldsymbol{H}(b,p_b) = \left(-\frac{1}{12l^3}\beta\frac{p_b^2}{b^2} + l^3\tilde{\Lambda}\beta^3\right)\mathbf{1}_{\mathrm{pert}} + \frac{1}{\beta}\sum_{k\in\Sigma}\omega_k(b)\boldsymbol{a}_k^*(b)\boldsymbol{a}_k(b). \tag{29}$$

Coming back to condition (C2), we recall that it requires $\boldsymbol{H}(b,p_b)$ to have a certain form. First, $\boldsymbol{H}(b,p_b)$ must be a bounded operator on the Fock space $\mathcal{F}_\mathrm{s}$. Besides, it should belong to one of the so-called symbol classes S^m_ρ. More precisely, the function itself and each of its derivatives must be bounded with respect to b and polynomially bounded with respect to p_b. In particular, there must be a positive constant $C_{\alpha,\delta}$ for every $\alpha,\delta \in \mathbb{N}$ such that for every p_b it holds true that

$$\sup_{b\in\mathbb{R}}\|(\partial_b^\alpha\partial_{p_b}^\beta\boldsymbol{H})(b,p_b)\|_{\mathcal{B}(\mathcal{F}_\mathrm{s})} \leq C_{\alpha,\delta}(1+p_b^2)^{\frac{1}{2}(m-\rho|\delta|)}. \tag{30}$$

$\boldsymbol{H}(b,p_b)$ fails to satisfy this condition *a priori* as it is not a bounded function with respect to b. A possible resort is to replace the Hamilton symbol by a bounded function above or below a certain energy value E_t and to truncate the sum over k in Eq. (29) to a fixed $N \in \mathcal{N}$. We performed such an analysis explicitly for a simple oscillator model in [11] and referred to this truncated version of the Hamilton symbol as the auxiliary Hamiltonian $\boldsymbol{H}_{\mathrm{aux}}$. We can apply the same strategy here and thereby guarantee that the auxiliary Hamiltonian is in $S^0_0(\Gamma_{\mathrm{hom}},\mathcal{B}(\mathcal{F}_\mathrm{s}))$. Unfortunately, the original Hamilton symbol is an *unbounded* operator on the fast Hilbert space, and it is hence not possible to reasonably compare the dynamics generated by this operator and the auxiliary structure mentioned before. We will hence remain with the original Hamiltonian when applying SAPT.

More generically, the symbol classes are Fréchet spaces with respective norms for the different values of m and ρ, and this allows one to neatly define a multiplication between the symbols and adjoints of them. The operator product on the space of Weyl operators transforms into a correspondent noncommutative "Moyal" or "star" product on the Fréchet spaces of symbol functions. With the rescaled momentum $p_b = \varepsilon P_b$, the Moyal product has here the form of a power series expansion in ε, and we consequently denote it by "$\star_\varepsilon$." This makes the space adiabatic perturbation scheme work at the technical level, and we are going to introduce its explicit form in Sec. III B. The third condition concerns the energy eigenvalues of the symbol Hamilton function $\boldsymbol{H}$.

$(\mathrm{C3})_\gamma$ *Gap condition*. For any fixed $(b,p_b) \in \mathbb{R}$, the spectrum $\sigma(b,p_b)$ of the Hamilton symbol $H(b,p_b)$ contains at least one isolated subset $\sigma_\nu(b,p_b)$ for some fixed quantum number(s) $\nu \in \mathbb{N}$ which is uniformly separated from the remainder $\sigma_{\mathrm{rem}} \coloneqq \sigma(b,p_b)\backslash\sigma_\nu(b,p_b)$. In particular, the minimal distance between the elements of σ_ν and the remainder is nonzero for every single $(b,p_b) \in \mathbb{R}^2$. More precisely, there exists an enclosing interval $I(b,p_b)$ for the relevant part of the spectrum $\sigma_\nu(b,p_b)$ such that for every value (b,p_b) the distance $\mathrm{dist}[\sigma_{\mathrm{rem}}(b,p_b),I(b,p_b)]$ is larger than or equal to $C_\mathrm{g}(1+p_b^2)^{\frac{\gamma}{2}}$, where $C_\mathrm{g} \geq 0$ is the "gap" constant and $\gamma \in \mathbb{R}$.

$\boldsymbol{H}(b,p_b)$ as given in (29) admits discrete energy bands as required by $(\mathrm{C3})_\gamma$. Indeed, the mode vectors k define a discrete set on the compact torus; when fixing (b,p_b) to certain values, there are discrete energy bands, and each of them has at least 2^3 degenerate eigenstates.

In order to analyze the corresponding Fock states, we start by defining the vacuum state $\Omega(b)$ and require that $\boldsymbol{a}_k(b)\Omega(b) = 0$ for every $k \in \Sigma$. Any excited eigenstate $\xi_{(n)}(b) \in \mathcal{F}_\mathrm{s}$ where (n) is a short form for the collection of its excitation numbers $\{n_{k,d_k}\}_{k\in\Sigma}$ with degeneracy numbers $d_k \in \mathbb{N}$ results from the (n)-times application of creation operators,

$$\xi_{(n)}(b) = \prod_{k\in\Sigma}\frac{(\boldsymbol{a}_k^*(b))^{n_k}}{\sqrt{n_k!}}\Omega(b). \tag{31}$$

The energy bands $E_{(n)}(b,p_b)$ are the (b,p_b)-dependent energy eigenvalues of the symbol function $\boldsymbol{H}(b,p_b)$ with respect to the excited eigenstates $\xi_{(n)}(b)$, such that

$$\boldsymbol{H}(b,p_b)\xi_{(n)}(b) = E_{(n)}(b,p_b)\xi_{(n)}(b), \tag{32}$$

$$\text{with}\quad E_{(n)}(b,p_b) = -\frac{1}{12l^3}\beta\frac{p_b^2}{b^2} + l^3\tilde{\Lambda}\beta^3 + \frac{1}{\beta}\sum_{n_k\in(n)}n_k\omega_k(b). \tag{33}$$

The spectrum of $\boldsymbol{H}(b,p_b)$ thus consists of the set of all energy bands, $\{E_{(n)}(b,p_b)\}_{(n)}$ for all possible combinations

of excitation numbers (n). SAPT demands one to choose an isolated subset $\sigma_\nu(b,p_b)\subset\sigma(b,p_b)$ which is uniformly separated from the remainder of the spectrum.

It appears that the energy function depends on (i) the norm $|k|$ of the wave vectors and (ii) their excitation numbers n_k for any of the excited one-particle states that contribute to the total Fock state. Obviously, these energy functions $E_{(n)}(b,p_b)$ are subject to eigenvalue crossings for varying (b,p_b). Such overlaps are prohibited for the application of SAPT. It is of course possible to identify domains within the homogeneous phase space in which we do not encounter such eigenvalue crossings. One can formally restrict the domain of the theory to such regions, but must adapt the whole quantization procedure for the homogeneous phase space. This will represent a very nontrivial task, but it is important since the whole scheme relies on the correct implementation of a phase space quantization within the homogeneous sector. This question must be explored elsewhere, and we focus here on the question of generic operability of the SAPT scheme.

The fourth and final condition for SAPT is the following:

(C4) *Convergence condition*. If the system satisfies the gap condition $(\mathrm{C3})_\gamma$ for some $\gamma\in\mathbb{R}$, the Hamilton symbol $\boldsymbol{H}(b,p_b)$ must be in S^γ_ρ. If $\rho=0$, γ must also vanish. If $\rho>0$, γ can be any real number but the Weyl quantization $\hat{\boldsymbol{H}}$ must be essentially self-adjoint on the Hilbert vector-valued Schwartz space, $\mathcal{S}(\mathbb{R},\mathcal{H}_\mathrm{f})$.

According to our discussion of the previous conditions, it will not be possible to strictly adhere to this condition for the given model such that we must abandon any of the convergence results of standard SAPT.

B. Perturbative construction scheme

The space adiabatic perturbation scheme divides into three steps and relies on the existence of the three following symbol functions. Given the Hamilton symbol $\boldsymbol{H}(b,p_b)\in S^0_0$, SAPT assures that [14]

(S1) there exists a formal symbol $\boldsymbol{\pi}=\sum_{i\geq0}\varepsilon^i\boldsymbol{\pi}_i$ with $\boldsymbol{\pi}_i\in S^0_0$ and such that $\boldsymbol{\pi}_0$ is the spectral projection of $\boldsymbol{H}(b,p_b)$ corresponding to $\sigma_\nu(b,p_b)$. We can construct $\boldsymbol{\pi}_{(I)}:=\sum_{i\leq I}\varepsilon^i\boldsymbol{\pi}_i$ up to order $I\in\mathbb{N}$ and with the properties

$$(\mathrm{S1\text{–}1})\quad \boldsymbol{\pi}_{(I)}\star_\varepsilon\boldsymbol{\pi}_{(I)}-\boldsymbol{\pi}_{(I)}=\mathcal{O}_0(\varepsilon^{I+1}),\tag{34}$$

$$(\mathrm{S1\text{–}2})\quad \boldsymbol{\pi}^*_{(I)}-\boldsymbol{\pi}_{(I)}=\mathcal{O}_0(\varepsilon^{I+1}),\tag{35}$$

$$(\mathrm{S1\text{–}3})\quad \boldsymbol{H}\star_\varepsilon\boldsymbol{\pi}_{(I)}-\boldsymbol{\pi}_{(I)}\star_\varepsilon\boldsymbol{H}=\mathcal{O}_0(\varepsilon^{I+1}).\tag{36}$$

It can be shown that the Weyl quantization of a formal resummation of $\boldsymbol{\pi}$ (see [10] for more details) is $\mathcal{O}_0(\varepsilon^\infty)$, close to a true projection operator $\hat{\boldsymbol{\Pi}}\in\mathcal{B}(\mathcal{H})$ that almost commutes with the Hamilton operator, i.e., $[\hat{\boldsymbol{H}},\hat{\boldsymbol{\Pi}}]=\mathcal{O}_0(\varepsilon^\infty)$. The estimate means that for all $m\in\mathbb{N}$, there exists a constant $C_m\geq0$ such that $\|[\hat{\boldsymbol{H}},\hat{\boldsymbol{\Pi}}]\|_{\mathcal{B}(\mathcal{H})}\leq C_m\varepsilon^m$.

(S2) Let $\boldsymbol{\pi}_\mathrm{p}\in S^0_0(\Gamma_\mathrm{hom},\mathcal{B}(\mathcal{H}_\mathrm{pert}))$ be the projection on some reference subspace $\mathcal{K}_\mathrm{pert}\subset\mathcal{H}_\mathrm{pert}$. We assume that there exists a symbol $\boldsymbol{u}_0\in S^0_0(\mathcal{B}(\mathcal{H}_\mathrm{pert}))$ such that $\boldsymbol{u}_0\cdot\boldsymbol{\pi}_0\cdot\boldsymbol{u}_0^*=\boldsymbol{\pi}_\mathrm{p}$ where "$\cdot$" denotes the operator product within $\mathcal{B}(\mathcal{H}_\mathrm{pert})$. Then, there is a formal symbol $\boldsymbol{u}=\sum_{i\geq0}\varepsilon^i\boldsymbol{u}_i$ such that its restriction to the Ith order $\boldsymbol{u}_{(I)}$ satisfies

$$(\mathrm{S2\text{–}1})\quad \boldsymbol{u}^*_{(I)}\star_\varepsilon\boldsymbol{u}_{(I)}-\mathbf{1}_\mathrm{pert}=\mathcal{O}_0(\varepsilon^{I+1}),\tag{37}$$

$$(\mathrm{S2\text{–}2})\quad \boldsymbol{u}_{(I)}\star_\varepsilon\boldsymbol{u}^*_{(I)}-\mathbf{1}_\mathrm{pert}=\mathcal{O}_0(\varepsilon^{I+1}),\tag{38}$$

$$(\mathrm{S2\text{–}3})\quad \boldsymbol{u}_{(I)}\star_\varepsilon\boldsymbol{\pi}_{(I)}\star_\varepsilon\boldsymbol{u}^*_{(I)}-\boldsymbol{\pi}_\mathrm{p}=\mathcal{O}_0(\varepsilon^{I+1}).\tag{39}$$

The construction of this almost unitary symbol has the purpose to map the dynamics of the Hamilton operator to a simpler subspace such that we can actually solve the dynamics on this simpler subspace. Therefore, we note that the Weyl quantized resummation of the symbol function $\boldsymbol{u}$ gives rise to a true unitary operator $\hat{\boldsymbol{U}}\in\mathcal{B}(\mathcal{H})$ which intertwines the projection operator $\hat{\boldsymbol{\Pi}}$ and $\hat{\boldsymbol{\pi}}_\mathrm{p}$ in the sense that $\hat{\boldsymbol{U}}\hat{\boldsymbol{\Pi}}\hat{\boldsymbol{U}}^\dagger=\hat{\boldsymbol{\pi}}_\mathrm{p}$ holds true.

(S3) The last step consists in constructing an "effective" Hamilton symbol $\boldsymbol{h}_\mathrm{eff}=\sum_{i\geq0}\varepsilon^i\boldsymbol{h}_{\mathrm{eff},i}$ or more precisely its restriction to the Ith order according to

$$\boldsymbol{h}_{\mathrm{eff},(I)}=\boldsymbol{u}_{(I)}\star_\varepsilon\boldsymbol{H}\star_\varepsilon\boldsymbol{u}^*_{(I)}.\tag{40}$$

For systems with an external time parameter t and the Weyl quantizations $\hat{\boldsymbol{u}}_{(I)}$ and $\hat{\boldsymbol{h}}_{\mathrm{eff},(I)}$ it holds true that

$$e^{-i\hat{\boldsymbol{H}}t}-\hat{\boldsymbol{u}}^\dagger_{(I)}e^{-i\hat{\boldsymbol{h}}_{\mathrm{eff},(I)}t}\hat{\boldsymbol{u}}_{(I)}=\mathcal{O}_0(\varepsilon^{I+1}|t|).\tag{41}$$

Hence, after unitarily transforming back to the original Hilbert space, the dynamics generated by $\hat{\boldsymbol{h}}_\mathrm{eff}$ corresponds "almost" to the dynamics of the original Hamilton operator $\hat{\boldsymbol{H}}$.

For further details about the construction scheme, we refer to the companion papers [10,11]. In the following, we are first going to construct $\boldsymbol{\pi}_{(1)}$ as well as $\boldsymbol{u}_{(1)}$ in order to finally determine $\boldsymbol{h}_{\mathrm{eff},(2)}$. Therefore, we recall that the perturbation parameter of the scheme is here provided by the dimensionless ratio of the coupling constants, namely $\varepsilon^2=\kappa/\lambda$. As we already rescaled the momentum P_b with a factor ε, the first perturbative orders of the Moyal product are given for two symbol functions $\boldsymbol{f}(b,p_b)\in S^{m_1}_\rho$, $\boldsymbol{g}(b,p_b)\in S^{m_2}_\rho$,

$$(\boldsymbol{f}\star_\varepsilon\boldsymbol{g})(b,p_b)=(\boldsymbol{f}\cdot\boldsymbol{g})(b,p_b)+\frac{i\varepsilon}{2}((\partial_b\boldsymbol{f})\cdot(\partial_{p_b}\boldsymbol{g})-(\partial_{p_b}\boldsymbol{f})\cdot(\partial_b\boldsymbol{g}))(b,p_b)+\mathcal{O}(\varepsilon^2).\tag{42}$$

To shorten the computations, it is reasonable to use the Poisson bracket notation $\{\boldsymbol{f},\boldsymbol{g}\}_{\mathrm{hom}} \coloneqq (\partial_b \boldsymbol{f})\cdot(\partial_{p_b}\boldsymbol{g}) - (\partial_{p_b}\boldsymbol{f})\cdot(\partial_b \boldsymbol{g})$. Let us then start to iteratively compute the Moyal projector.

1. Construction of the projector symbol $\boldsymbol{\pi}_{(1)}$

To construct the symbol function $\boldsymbol{\pi}_{(1)} = \boldsymbol{\pi}_0 + \varepsilon\boldsymbol{\pi}_1$, we start by defining the zeroth order symbol $\boldsymbol{\pi}_0$. According to the construction step (S1), $\boldsymbol{\pi}_0(b)$ corresponds to the spectral projection of $\boldsymbol{H}(b,p_b)$ onto one of its energy bands $\sigma_\nu(b,p_b)$. In particular, we choose $\boldsymbol{\pi}_0$ to be defined as

$$\boldsymbol{\pi}_0(b) = \sum_{d=1}^{D_\nu} \xi_{(\nu)_d}(b)\langle \xi_{(\nu)_d}(b),\cdot\rangle_{\mathcal{F}_s}, \tag{43}$$

where $(\nu)_d = \{\nu_{k,d}\}_{k\in\Sigma}$ is the set of excitation numbers of the chosen Fock state and $d = 1,\ldots,D_\nu$ is the associated degeneracy label. Note that it solely depends on the configuration variable b and not on the momentum p_b. The projector symbol $\boldsymbol{\pi}_0(b)$ exists for every point $(b,p_b) \in \Gamma_{\mathrm{hom}}$ for which the energy gap between $E_{(\nu)}(b,p_b)$ and the remainder of the spectrum persists. Because of the continuity of the map $(b,p_b)\mapsto \boldsymbol{H}(b,p_b)$, also $(b,p_b)\mapsto\boldsymbol{\pi}_0(b)$ is continuous. By construction, $\boldsymbol{\pi}_0$ satisfies the construction rules (S1) restricted to the zeroth order in ε. In particular, it satisfies the conditions (S1–1) $\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_0 - \boldsymbol{\pi}_0 = 0$, (S1–2) $\boldsymbol{\pi}_0^* = \boldsymbol{\pi}_0$, and (S1–3) $[\boldsymbol{H},\boldsymbol{\pi}_0] = 0$. Consequently, the symbol (43) satisfies the base clause for the inductive construction scheme.

The next perturbative order of the rules (S1) serves to determine the first order symbol $\boldsymbol{\pi}_1$. By means of the Moyal product expansion (42), the rule (S1–1) restricted to its first order components provides an equation for determining the diagonal parts of $\boldsymbol{\pi}_1$, namely

$$\frac{i}{2}\{\boldsymbol{\pi}_0,\boldsymbol{\pi}_0\}_{\mathrm{hom}} + \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1 + \boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0 = \boldsymbol{\pi}_1. \tag{44}$$

The Poisson bracket vanishes as $\boldsymbol{\pi}_0$ solely depends on b. This implies that the diagonal contributions $\boldsymbol{\pi}_1^{\mathrm{D},0} \coloneqq \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}^{\mathrm{D},\perp} = \boldsymbol{\pi}_0^\perp\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0^\perp$ vanish, too. Here, we introduced the orthogonal complement of $\boldsymbol{\pi}_0$, namely $\boldsymbol{\pi}_0^\perp \coloneqq \mathbf{1}_{\mathrm{pert}} - \boldsymbol{\pi}_0$. As discussed in the companion paper [10], the construction rule (S1–3) provides the off-diagonal part of $\boldsymbol{\pi}_1$. Its restriction to the first order in ε is given by

$$\frac{1}{2}\{\boldsymbol{H},\boldsymbol{\pi}_0\}_{\mathrm{hom}} - \frac{1}{2}\{\boldsymbol{\pi}_0,\boldsymbol{H}\}_{\mathrm{hom}} + \boldsymbol{H}\cdot\boldsymbol{\pi}_1 - \boldsymbol{\pi}_1\cdot\boldsymbol{H} = 0. \tag{45}$$

We extract the off-diagonal contributions $\boldsymbol{\pi}_1^{\mathrm{OD},1} \coloneqq \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0^\perp$ and $\boldsymbol{\pi}_1^{\mathrm{OD},2} \coloneqq \boldsymbol{\pi}_0^\perp\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0$ by multiplying Eq. (45) with $\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}_0^\perp$ from the left and the right, respectively, and vice versa. We define the orthogonal part of $\boldsymbol{H}$ by $\boldsymbol{H}^\perp \coloneqq \boldsymbol{H}\cdot\boldsymbol{\pi}_0^\perp$, and we use that $\boldsymbol{H}\cdot\boldsymbol{\pi}_0 = E_{(\nu)}\mathbf{1}_{\mathrm{pert}}$. This yields for the total symbol $\boldsymbol{\pi}_1 = \boldsymbol{\pi}_1^{\mathrm{OD},1} + \boldsymbol{\pi}_1^{\mathrm{OD},2}$

$$\begin{aligned}\boldsymbol{\pi}_1 = -\frac{i}{2}&(\boldsymbol{\pi}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{H}+E_{(\nu)}\mathbf{1}_{\mathrm{pert}}\}_{\mathrm{hom}}\cdot(\boldsymbol{H}^\perp - E_{(\nu)}\mathbf{1}_{\mathrm{pert}})^{-1}\cdot\boldsymbol{\pi}_0^\perp \\ &+ (\boldsymbol{H}^\perp - E_{(\nu)}\mathbf{1}_{\mathrm{pert}})^{-1}\cdot\boldsymbol{\pi}_0^\perp\cdot\{\boldsymbol{\pi}_0,\boldsymbol{H}+E_{(\nu)}\mathbf{1}_{\mathrm{pert}}\}_{\mathrm{hom}}\cdot\boldsymbol{\pi}_0).\end{aligned} \tag{46}$$

For a concrete evaluation of $\boldsymbol{\pi}_1$, it is necessary to evaluate the derivatives of the eigenfunctions $\xi_n(b)$ with respect to b. Therefore, we use the explicit b-dependence of the creation operators $\boldsymbol{a}_k^*(b)$ in line with Eq. (28) and relation (31) for the excited Fock states. Let us first define the function

$$f_k(b) \coloneqq -\frac{1}{4}\frac{\partial_b\omega_k(b)}{\omega_k(b)}. \tag{47}$$

Then, the identity $\partial_b\boldsymbol{a}_k(b) = -2f_k(b)\boldsymbol{a}_k^*(b)$ follows from Eq. (28), and together with $\boldsymbol{a}_k(b)\Omega(b) = 0,\ \forall\ k\in\Sigma$, it implies that the derivative of the vacuum state $\Omega(b)$ is given by

$$\frac{\partial\Omega(b)}{\partial b} = \sum_{k\in\Sigma} f_k(b)\boldsymbol{a}_k^*(b)\boldsymbol{a}_k^*(b)\Omega(b). \tag{48}$$

Given the derivatives of the creation operators and the vacuum state, it is straightforward to infer from Eq. (31) the derivative of the excited state $\xi_{(\nu)_d}(b)$. Therefore, we denote the state whose quantum number $\nu_{k,d}$ for the wave vector k is shifted by ±2 compared to the state $\xi_{(\nu)_d}(b)$ by $\xi_{\{\ldots,\nu_{k,d}\pm2,\ldots\}}$. Then, the derivative of $\xi_{(\nu)_d}(b)$ is given by

$$\begin{aligned}\frac{\partial\xi_{(\nu)_d}(b)}{\partial b} &= -\sum_{k\in\Sigma} f_k(b)\sqrt{(\nu_{k,d}-1)\nu_{k,d}}\frac{(\boldsymbol{a}_k^*)^{\nu_{k,d}-2}}{\sqrt{(\nu_{k,d}-2)!}}\prod_{m\in\Sigma\setminus\{k\}}\frac{(\boldsymbol{a}_m^*)^{\nu_{m,d}}}{\sqrt{\nu_{m,d}!}}\Omega(b) \\ &\quad + \sum_{k\in\Sigma} f_k(b)\sqrt{(\nu_{k,a}+1)(\nu_{k,d}+2)}\frac{(\boldsymbol{a}_k^*)^{\nu_{k,d}+2}}{\sqrt{(\nu_{k,d}+2)!}}\prod_{m\in\Sigma\setminus\{k\}}\frac{(\boldsymbol{a}_m^*)^{\nu_{m,d}}}{\sqrt{\nu_{m,d}!}}\Omega(b) \\ &= \sum_{k\in\Sigma} f_k(b)[-\sqrt{(\nu_{k,d}-1)\nu_{k,d}}\xi_{\{\ldots,\nu_{k,d}-2,\ldots\}} + \sqrt{(\nu_{k,d}+1)(\nu_{k,d}+2)}\xi_{\{\ldots,\nu_{k,d}+2,\ldots\}}].\end{aligned} \tag{49}$$

The b-derivative of any Hilbert space vector in $\mathcal{H}_{\text{pert}}$ actually corresponds to a covariant derivative in the following sense. Consider the slow, homogeneous phase space Γ_{hom} as the base manifold of some infinite dimensional Hilbert bundle and let $\mathcal{F}_{\text{s}}(b, p_b)$ be the fiber space associated with a point $(b, p_b) \in \Gamma_{\text{hom}}$. Correspondingly, the derivative with respect to b is a standard covariant derivative $\boldsymbol{\mathcal{A}}(b):\Gamma(\mathcal{H}_{\text{pert}}) \to \Gamma(\mathcal{H}_{\text{pert}})$ on the space of Hilbert bundle sections $\Gamma(\mathcal{H}_{\text{pert}})$ of the total Hilbert bundle. With the choice of the basis states $\{\xi_{(n)}\}$, we write for $\boldsymbol{\mathcal{A}}(b)$ with respect to this basis,

$$\boldsymbol{\mathcal{A}}_{(n)_d}^{(m)_c} = \sum_{k\in\Sigma} f_k \Big(-\sqrt{n_{k,d}(n_{k,d}-1)}\,\delta_{(n)}^{\{\ldots,m_{k,c}+2,\ldots\}} + \sqrt{(n_{k,d}+2)(n_{k,d}+1)}\,\delta_{(n)}^{\{\ldots,m_{k,c}-2,\ldots\}} \Big),$$

where d and c are the degeneracy labels for the excitation numbers (n) and (m). In summary, the derivative of the state $\xi_{(\nu)_d}(b)$ can be written using the entries $\mathcal{A}$ of the covariant derivative

$$\frac{\partial \xi_{(\nu)_d}(b)}{\partial b} = \sum_{k\in\Sigma} \big(\mathcal{A}_{(n)_d}^{\{\ldots,n_{k,d}-2,\ldots\}} \xi_{\{\ldots,n_{k,d}-2,\ldots\}} + \mathcal{A}_{(n)_d}^{\{\ldots,n_{k,d}+2,\ldots\}} \xi_{\{\ldots,n_{k,d}+2,\ldots\}} \big). \tag{50}$$

As a consequence, the b-derivative of the projector symbol $\boldsymbol{\pi}_0(b)$ results from the functional representation of the projector due to Riesz (43),

$$\begin{aligned}\frac{\partial \boldsymbol{\pi}_0(b)}{\partial b} = \sum_{d=1}^{D_\nu} \sum_{k\in\Sigma} \big(& \mathcal{A}_{(\nu)_d}^{\{\ldots,\nu_{k,d}-2,\ldots\}} \big(\xi_{(\nu)_d} \langle \xi_{\{\ldots,\nu_{k,d}-2,\ldots\}}, \cdot \rangle_{\mathcal{F}_{\text{s}}} + \xi_{\{\ldots,\nu_{k,d}-2,\ldots\}} \langle \xi_{(\nu)_d}, \cdot \rangle_{\mathcal{F}_{\text{s}}} \big) \\ & + \mathcal{A}_{(\nu)_d}^{\{\ldots,\nu_{k,d}+2,\ldots\}} \big(\xi_{(\nu)_d} \langle \xi_{\{\ldots,\nu_{k,d}+2,\ldots\}}, \cdot \rangle_{\mathcal{F}_{\text{s}}} + \xi_{\{\ldots,\nu_{k,d}+2,\ldots\}} \langle \xi_{(\nu)_d}, \cdot \rangle_{\mathcal{F}_{\text{s}}} \big) \big).\end{aligned} \tag{51}$$

With this, we can evaluate the symbol $\boldsymbol{\pi}_1$ according to Eq. (46). The Poisson bracket in this equation also requires one to determine the p_b-derivative of the symbol function $\boldsymbol{H} + E_{(\nu)}\mathbf{1}_{\text{pert}}$. On the one hand, the homogeneous, gravitational part of the Hamilton symbol $\boldsymbol{H}$ depends on p_b, and so does $E_{(\nu)}$. The respective part is proportional to the unity operator with proportionality factor

$$E_{\text{hom}}(b, p_b) = -\frac{1}{12l^3}\beta(b, p_b)\frac{p_b^2}{b^2} + l^3\tilde{\Lambda}\beta(b, p_b)^3. \tag{52}$$

Besides, the perturbative field contribution of the Hamilton symbol depends on p_b via the global prefactor $\beta(b, p_b)^{-1}$; cf. Eq. (29) such that diagonal contributions from this part enter as well in the evaluation of the Poisson bracket. We denote the perturbative part of $E_{(\nu)}$ as $E_{\text{pert},(\nu)}$. To determine these contributions let us consider the first line in the equation for $\boldsymbol{\pi}_1$, Eq. (46), and thereby start from the left. The multiplication of $\boldsymbol{\pi}_0$ from the left to $\partial_b\boldsymbol{\pi}_0$ selects the two suitable contributions in (51). Consequently, there are only two relevant contributions in $\partial_{p_b}(\boldsymbol{H} + E_{(\nu)}\mathbf{1}_{\text{pert}})$ for every $k \in \Sigma$ that enter the game. Moving on to the right side of the first line, these two terms preselect two of the entries of $(\boldsymbol{H}^{\perp} - E_{(\nu)}\mathbf{1}_{\text{pert}})^{-1}$ for every k: $(E_{\{\ldots,\nu_{k,d}-2,\ldots\}} - E_{(\nu)})\xi_{\{\ldots,\nu_{k,d}-2,\ldots\}} \langle \xi_{\{\ldots,\nu_{k,d}-2,\ldots\}}, \cdot \rangle_{\mathcal{F}_{\text{s}}}$ and $(E_{\{\ldots,\nu_{k,d}+2,\ldots\}} - E_{(\nu)})\xi_{\{\ldots,\nu_{k,d}+2,\ldots\}} \langle \xi_{\{\ldots,\nu_{k,d}+2,\ldots\}}, \cdot \rangle_{\mathcal{F}_{\text{s}}}$. The two scalars evaluate to $\mp\Delta_k := \mp\frac{2}{\beta}\omega_k(b)$. The second line unfolds in the same way such that $\boldsymbol{\pi}_1$ in explicit form is given by

$$\begin{aligned}\boldsymbol{\pi}_1 = \frac{i}{2}\sum_{d=1}^{D_\nu}\sum_{k\in\Sigma} \big(& \mathcal{A}_{(\nu)_d}^{\{\ldots,\nu_{k,d}-2,\ldots\}} C_{1,(\nu),k} \big(\xi_{(\nu)_d} \langle \xi_{\{\ldots,\nu_{k,d}-2,\ldots\}}, \cdot \rangle_{\mathcal{F}_{\text{s}}} - \xi_{\{\ldots,\nu_{k,d}-2,\ldots\}} \langle \xi_{(\nu)_d}, \cdot \rangle_{\mathcal{F}_{\text{s}}} \big) \\ & + \mathcal{A}_{(\nu)_d}^{\{\ldots,\nu_{k,d}+2,\ldots\}} C_{2,(\nu),k} \big(\xi_{(\nu)_a} \langle \xi_{\{\ldots,\nu_{k,d}+2,\ldots\}}, \cdot \rangle_{\mathcal{F}_{\text{s}}} - \xi_{\{\ldots,\nu_{k,d}+2,\ldots\}} \langle \xi_{(\nu)_d}, \cdot \rangle_{\mathcal{F}_{\text{s}}} \big) \big),\end{aligned} \tag{53}$$

where we defined the functions $C_{1,(\nu),k}(b, p_b)$ and $C_{2,(\nu),k}(b, p_b)$ according to

$$C_{1,(\nu),k}(b, p_b) := \frac{1}{\Delta_k}\left(\frac{\partial E_{\text{hom}}}{\partial p_b} - \frac{1}{\beta}\frac{\partial \beta}{\partial p_b} E_{\text{pert},(\nu)} \right) + \frac{1}{\beta}\frac{\partial \beta}{\partial p_b}, \tag{54}$$

$$C_{2,(\nu),k}(b, p_b) := -\frac{1}{\Delta_k}\left(\frac{\partial E_{\text{hom}}}{\partial p_b} - \frac{1}{\beta}\frac{\partial \beta}{\partial p_b} E_{\text{pert},(\nu)} \right) + \frac{1}{\beta}\frac{\partial \beta}{\partial p_b}. \tag{55}$$

For the final construction rule, (S1–2), it is easy to check that $\boldsymbol{\pi}_{(1)}$ indeed equals $\boldsymbol{\pi}_{(1)}^*$ by simply transposing and complex conjugating our results for $\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}_1$. For closing this subsection, we emphasize that the Weyl quantization of the Moyal projector $\boldsymbol{\pi}_{(1)}$ is a very nontrivial operator on the total Hilbert space $\mathcal{H}$ due to the dependence of $\boldsymbol{\pi}_{(1)}$ on (b, p_b) and ε. SAPT therefore suggests to construct a Moyal unitary symbol $\boldsymbol{u}$ which maps the dynamical subspace related to $\boldsymbol{\pi}$ or more precisely here to $\boldsymbol{\pi}_{(1)}$ to a suitable reference subspace $\mathcal{K}_{\text{pert}} \subset \mathcal{H}_{\text{pert}}$.

2. Construction of the Moyal unitary $\boldsymbol{u}_{(1)}$

We choose an arbitrary but suitable reference subspace $\mathcal{K}_{\text{pert}} \subset \mathcal{H}_{\text{pert}}$ to which we map the relevant dynamics of the problem. The idea is to select one fixed point $(b_0, p_{b,0}) \in \Gamma_{\text{hom}}$. We denote the eigenbasis of $\boldsymbol{H}(b_0, p_{b,0})$ by $\{\zeta_{(n)}\} := \{\xi_{(n)}(b_0)\}$, and we define the reference projection as

$$\boldsymbol{\pi}_{\mathrm{p}} \coloneqq \sum_{d=1}^{D_\nu} \zeta_{(\nu)_d} \langle \zeta_{(\nu)_d}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{56}$$

We denote the subspace associated with the projection symbol $\boldsymbol{\pi}_{\mathrm{p}}$ by $\mathcal{K}_{\mathrm{pert}}$ as outlined before. In order to mediate between $\boldsymbol{\pi}\mathcal{H}_{\mathrm{pert}}$ and $\mathcal{K}_{\mathrm{pert}}$, and vice versa, a unitary symbol function $\boldsymbol{u}(b, p_b)$ is necessary. The space adiabatic scheme assumes the symbol to have the form of a formal power series in ε. We restrict its computation to the first order $\boldsymbol{u}_{(1)} = \boldsymbol{u}_0 + \varepsilon \boldsymbol{u}_1$, and we define its zeroth order component to be

$$\boldsymbol{u}_0(b) \coloneqq \sum_{(n)} \sum_{d=1}^{D_{(n)}} \zeta_{(n)_d} \langle \xi_{(n)_d}(b), \cdot \rangle_{\mathcal{F}_{\mathrm{s}}}, \tag{57}$$

where the sum over (n) is a sum over all possible combinations of excitation numbers in the field Fock space. It is straightforward to show that $\boldsymbol{u}_0$ and $\boldsymbol{\pi}_{\mathrm{p}}$ together with $\boldsymbol{\pi}_0$ satisfy the base clause of the construction rules (S2), namely (S2–1) $\boldsymbol{u}_0^* \cdot \boldsymbol{u}_0 = \mathbf{1}_{\mathrm{pert}}$, (S2–2) $\boldsymbol{u}_0 \cdot \boldsymbol{u}_0^* = \mathbf{1}_{\mathrm{pert}}$, and (S2–3) $\boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}_0^* = \boldsymbol{\pi}_{\mathrm{p}}$. For the construction of $\boldsymbol{u}_1$, it is useful to split $\boldsymbol{u}_1$ into a Hermitian and an anti-Hermitian part, $\boldsymbol{a}_1 = \boldsymbol{a}_1^*$ and $\boldsymbol{b}_1 = -\boldsymbol{b}_1^*$ such that $\boldsymbol{u}_1 =: (\boldsymbol{a}_1 + \boldsymbol{b}_1) \cdot \boldsymbol{u}_0$. The construction rule (S2–1) serves to determine $\boldsymbol{a}_1$ for our choice of $\boldsymbol{\pi}_{\mathrm{p}}$ and $\boldsymbol{u}_0$. In particular, its restriction to first order is given by

$$\frac{i}{2}\{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_{\mathrm{hom}} + 2\boldsymbol{a}_1 = 0. \tag{58}$$

As a consequence, we have that $\boldsymbol{a}_1 = 0$; i.e., there are no Hermitian contributions to $\boldsymbol{u}_1$. To determine the remaining anti-Hermitian piece, let us consider the construction rule (S2–3), again restricted to first order in ε,

$$[\boldsymbol{b}_1, \boldsymbol{\pi}_{\mathrm{p}}]_{\mathrm{pert}} + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1 \cdot \boldsymbol{u}_0^* = 0. \tag{59}$$

We then use that $\boldsymbol{b}_1 = -[\boldsymbol{\pi}_{\mathrm{p}}, [\boldsymbol{b}_1, \boldsymbol{\pi}_{\mathrm{p}}]_{\mathrm{pert}}]_{\mathrm{pert}}$ provides a solution for $\boldsymbol{b}_1$ which simply evaluates to

$$\boldsymbol{u}_1 = [\boldsymbol{\pi}_{\mathrm{p}}, \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1 \cdot \boldsymbol{u}_0^*]_{\mathrm{pert}} \cdot \boldsymbol{u}_0. \tag{60}$$

With the solution of $\boldsymbol{\pi}_1$ in Eq. (53), this gives the following result for $\boldsymbol{u}_1$:

$$\begin{aligned}\boldsymbol{u}_1 = \frac{i}{2} \sum_{d=1}^{D_\nu} \sum_{k \in \Sigma} \big(& \mathcal{A}_{(\nu)_d}^{\{\ldots,\nu_{k,d}-2,\ldots\}} C_{1,(\nu),k} \big(\zeta_{(\nu)_d} \langle \xi_{\{\ldots,\nu_{k,d}-2,\ldots\}}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}} \\ & + \zeta_{\{\ldots,\nu_{k,a}-2,\ldots\}} \langle \xi_{(\nu)_d}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}} \big) \\ & + \mathcal{A}_{(\nu)_d}^{\{\ldots,\nu_{k,d}+2,\ldots\}} C_{2,(\nu),k} \big(\zeta_{(\nu)_d} \langle \xi_{\{\ldots,\nu_{k,d}+2,\ldots\}}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}} \\ & + \zeta_{\{\ldots,\nu_{k,d}+2,\ldots\}} \langle \xi_{(\nu)_d}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}} \big) \big). \end{aligned} \tag{61}$$

3. Construction of the effective Hamiltonian $\boldsymbol{h}_{\mathbf{eff},(2)}$

The last step of the perturbation scheme consists in pulling the dynamics of the chosen subspace associated with the Weyl quantization of $\boldsymbol{\pi}$ to the ε-independent subspace $\hat{\boldsymbol{\pi}}_{\mathrm{p}}\mathcal{H}_{\mathrm{pert}}$. The effective Hamilton operator $\hat{\boldsymbol{h}}_{\mathrm{eff}}$ acting on this subspace is the Weyl quantization of the symbol function $\boldsymbol{h}_{\mathrm{eff}}$ which obeys the construction rule (S3), namely $\boldsymbol{h}_{\mathrm{eff}} = \boldsymbol{u} \star_\varepsilon \boldsymbol{H} \star_\varepsilon \boldsymbol{u}^*$. Again, we assume a power series ansatz with respect to ε for the symbol $\boldsymbol{h}_{\mathrm{eff}}$ that we are going to determine up to second order, i.e., $\boldsymbol{h}_{\mathrm{eff},(1)} = \boldsymbol{h}_{\mathrm{eff},0} + \varepsilon \boldsymbol{h}_{\mathrm{eff},1} + \varepsilon^2 \boldsymbol{h}_{\mathrm{eff},2}$. In the following, we restrict our attention to the dynamics within the relevant subspace and thus project $\boldsymbol{h}_{\mathrm{eff},(2)}$ on $\boldsymbol{\pi}_{\mathrm{p}}$. The restriction to the zeroth order of (S3) yields

$$\begin{aligned}\boldsymbol{h}_{\mathrm{eff},0,\mathrm{p}}(b, p_b) &\coloneqq \boldsymbol{\pi}_{\mathrm{p}} \cdot \boldsymbol{u}_0 \cdot \boldsymbol{H} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\mathrm{p}} \\ &= \left(-\frac{1}{12 l^3} \beta \frac{p_b^2}{b^2} + l^3 \tilde{\Lambda} \beta^3 + \frac{1}{\beta} \sum_{k \in \Sigma} \omega_k(b) \nu_k \right) \boldsymbol{\pi}_{\mathrm{p}}. \end{aligned} \tag{62}$$

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, homogeneous part $E_{\mathrm{hom}}(b, p_b)$, but also the backreaction contribution from the Klein-Gordon energy band (ν) that has been chosen.

For the first and second order contributions of $\boldsymbol{h}_{\mathrm{eff}}$, it is useful to star multiply the condition (S3) by $\boldsymbol{u}$ from the right such that the double star product does not have to be carried out. The restriction of the resulting equation to the first order in ε yields (cf. [11,15])

$$\begin{aligned}\boldsymbol{h}_{\mathrm{eff},1} = \Big(& \boldsymbol{u}_1 \cdot \boldsymbol{H} - \boldsymbol{h}_{\mathrm{eff},0} \cdot \boldsymbol{u}_1 + \frac{i}{2} \{\boldsymbol{u}_0, \boldsymbol{H}\}_{\mathrm{hom}} \\ & - \frac{i}{2} \{\boldsymbol{h}_{\mathrm{eff},0}, \boldsymbol{u}_0\}_{\mathrm{hom}} \Big) \cdot \boldsymbol{u}_0^*. \end{aligned} \tag{63}$$

To evaluate $\boldsymbol{h}_{\mathrm{eff},1}$, recall that $\boldsymbol{u}_1$ has no diagonal contributions according to (61), and that $\boldsymbol{u}_0$ is independent of p_b. Therefore, $\boldsymbol{h}_{\mathrm{eff},1}$ has no diagonal contributions at all such that $\boldsymbol{h}_{\mathrm{eff},1,\mathrm{p}} \coloneqq \boldsymbol{\pi}_{\mathrm{p}} \cdot \boldsymbol{h}_{\mathrm{eff},1} \cdot \boldsymbol{\pi}_{\mathrm{p}}$ vanishes identically. The same strategy for determining $\boldsymbol{h}_{\mathrm{eff},1,\mathrm{p}}$ applies for deriving $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}$. Together with the fact that $\boldsymbol{u}_0$ only depends on b and not on p_b, it yields

$$\begin{aligned}\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}} = \boldsymbol{\pi}_{\mathrm{p}} \cdot \Big[& \frac{i}{2} \big(\{\boldsymbol{u}_1, \boldsymbol{H} + E_{(\nu)} \mathbf{1}_{\mathrm{pert}}\}_{\mathrm{hom}} \\ & - \{\boldsymbol{h}_{\mathrm{eff},1}, \boldsymbol{u}_0\}_{\mathrm{hom}} \big) - \boldsymbol{h}_{\mathrm{eff},1} \cdot \boldsymbol{u}_1 \Big] \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\mathrm{p}}. \end{aligned} \tag{64}$$

Note that $\boldsymbol{h}_{\mathrm{eff},1}$ is nonvanishing, in contrast to $\boldsymbol{h}_{\mathrm{eff},1,\mathrm{p}}$, and its nonvanishing contributions need *a priori* to be taken into

account in the evaluation of $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}$. Nevertheless, it can be shown that the second and the third terms involving $\boldsymbol{h}_{\mathrm{eff},1}$ vanish identically [10]. In particular, it holds true that $\boldsymbol{\pi}_{\mathrm{p}} \cdot \boldsymbol{h}_{\mathrm{eff},1} = 0$ due to symmetry reasons. By pulling the symbol $\boldsymbol{\pi}_{\mathrm{p}}$ into the Poisson bracket of the second term, which is allowed since $\boldsymbol{\pi}_{\mathrm{p}}$ is independent of b and p_b, also the second term vanishes. Thus, the evaluation of $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}$ is confined to the first contribution. Using the result for $\boldsymbol{u}_1$ in Eq. (61) yields *a priori* for the second order contribution of the effective Hamilton symbol

$$\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}} = \sum_{d=1}^{D_\nu}\left[\sum_{k\in\Sigma}\left(\frac{C_{3,(\nu)}}{\omega_k^3}\left(\nu_{k,d}+\frac{1}{2}\right)+\frac{C_{4,(\nu)}}{\omega_k^4}(\nu_{k,d}^2+\nu_{k,d}+1)+\frac{C_{5,(\nu)}}{\omega_k^5}\left(\nu_{k,d}+\frac{1}{2}\right)\right)\right]\cdot\zeta_{(\nu)_d}\langle\zeta_{(\nu)_d},\cdot\rangle_{\mathcal{F}_{\mathrm{s}}}, \tag{65}$$

where we employed the phase space functions $C_{3,(\nu)}(b,p_b)$, $C_{4,(\nu)}(b,p_b)$, and $C_{5,(\nu)}(b,p_b)$,

$$C_{3,(\nu)}(b,p_b) \coloneqq \frac{\mu^4 b^2}{8}\left(\frac{1}{\beta^3}\left(\frac{\partial\beta}{\partial p_b}\right)^2-\frac{1}{\beta^2}\left(\frac{\partial^2\beta}{\partial p_b^2}\right)\right) = -\frac{\sigma^2\mu^4 b^2}{8\beta^5}, \tag{66}$$

$$C_{4,(\nu)}(b,p_b) \coloneqq \frac{\mu^4 b^2}{16}\left(\frac{2}{\beta}\frac{\partial\beta}{\partial p_b}\frac{\partial E_{\mathrm{hom}}}{\partial p_b}+\frac{\partial^2 E_{\mathrm{hom}}}{\partial p_b^2}-\frac{1}{\beta}\frac{\partial^2\beta}{\partial p_b^2}E_{\mathrm{pert},(\nu)}\right), \tag{67}$$

$$C_{5,(\nu)} \coloneqq \frac{\mu^4 b^2}{8}\left(2\frac{\partial\beta}{\partial p_b}\frac{\partial E_{\mathrm{hom}}}{\partial p_b}E_{\mathrm{pert},(\nu)}-\beta\left(\frac{\partial E_{\mathrm{hom}}}{\partial p_b}\right)^2-\frac{1}{\beta}\left(\frac{\partial\beta}{\partial p_b}\right)^2 E_{\mathrm{pert},(\nu)}^2\right). \tag{68}$$

Note that these functions do not depend on the wave vector k which has been employed as a summation index in (65). 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 ε. In particular, it is clear from the definitions (21) that σ is proportional to ε, and hence the terms including derivatives of $\beta = (b^2+\sigma^2\frac{p_b^2}{b^2})^{1/2}$ with respect to p_b contribute additional factors of ε. The remaining terms at second order are

$$\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}|_{\varepsilon^2} = -\frac{3\mu^4 l^3}{32}\sum_{d=1}^{D_\nu}\zeta_{(\nu)_d}\langle\zeta_{(\nu)_d},\cdot\rangle_{\mathcal{F}_{\mathrm{s}}}\cdot\sum_{k\in\Sigma}\left(\frac{b^4}{\beta^3}\frac{1}{\omega_k^4}(\nu_{k,d}^2+\nu_{k,d}+1)+\frac{3l^3p_b^2b^2}{\beta}\frac{1}{\omega_k^5}\left(\nu_{k,d}+\frac{1}{2}\right)\right).$$

We emphasize that the sums over all modes k in this expression converge. First, the integers $\nu_{k,d}$ are only nonvanishing for a finite number of modes k which solves the convergence problem for terms which enter with polynomials of $\nu_{k,d}$. The remaining constant contributions, however, benefit from the high inverse order of $\omega_k = \sqrt{k^2+\mu^2 b^2}$ that enters. It is thus possible to explicitly compute the effective Hamilton symbol up to second order in ε for the cosmological field model, and we obtain a convergent result albeit the sum over all the modes. In the next step, and we leave this for a further publication, the aim is to find solutions with respect to the nontrivial slow scalar part of $\boldsymbol{h}_{\mathrm{eff},(2),\mathrm{p}}$. The application of the operator $\hat{\boldsymbol{u}}$ then yields wave functions in $\mathcal{H}$ which are exact solutions up to errors of order ε^3 as shown in [10].

IV. CONCLUSION AND OUTLOOK

In this paper, we computed an effective Hamiltonian that incorporates the influence of the inhomogeneous degrees of freedom on the quantum dynamics of the homogeneous variables. This was realized for every energy band associated with an excited state of the inhomogeneous cosmological Fock state separately. It is possible to compute the spectrum of these effective Hamiltonians. By rotating the corresponding (possibly generalized) eigenvectors by the approximate inverse unitary operator that was used to achieve the adiabatic decoupling of the energy bands, one obtains approximate eigenvectors of the original Hamiltonian. The latter includes 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) generalized energy basis in order to study their quantum evolution and in particular the possible fate of the classical big bang singularity. We reserve this for future work.

In the final paper [12] of this series, we consider general relativity without dust coupled to a real-valued Klein-Gordon scalar field. We start from the formulation of the dynamics in terms of the canonical variables used for the hybrid quantization scheme [25,26]. These are already ideally suited for an application of the space adiabatic

perturbation scheme. The challenge is twofold: First, the dependence of the inhomogeneous 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 difficult. 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 detailed discussion.

ACKNOWLEDGMENTS

S. S. thanks the Heinrich Böll Foundation e.V. for financial and intellectual support and the German Academic Scholarship Foundation for intellectual support.

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