Quantum cosmological backreactions. IV. Constrained quantum cosmological perturbation theory

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This is the final paper in a series of four in which we incorporate backreaction among the homogeneous and between the homogeneous and inhomogeneous degrees of freedom in quantum cosmological perturbation theory using space adiabatic methods. Here, we consider the gauge-invariant scalar (Mukhanov-Sasaki) and tensor (primordial gravitational wave) perturbations of general relativity coupled to a scalar field which arise from a careful constraint analysis of this system up to second order in the perturbations. The simultaneous quantization of the homogeneous and inhomogeneous degrees of freedom requires the use of a suitable constructive perturbation scheme for which we employ space adiabatic perturbation theory, a rigorous extension of the standard Born-Oppenheimer theory. We are confronted with several challenges arising for theories with an infinite number of degrees of freedom. We are able to compute the backreaction effects up to second order in the adiabatic parameter and find modifications as compared to earlier derivations of the effective quantum dynamics of the homogeneous sector.

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I. INTRODUCTION

The present paper represents the culmination of a series of four papers [1–3] in which we use space adiabatic perturbation theory (SAPT) [4,5] together with the hybrid approach to quantum cosmology [6] in order to capture quantum backreaction effects between the homogeneous and inhomogeneous degrees of freedom of both matter and geometry. In summary, we aim at describing the earliest moments of the Universe, based on the premise that the Universe should be described in its entirety by a theory of quantum gravity back then. Since we do not have a complete theory of quantum gravity at our disposal (despite the numerous promising approaches in this direction such as asymptotic safety [7–10], string theory, in particular in its ADS/CFT incarnation [11,12], causal dynamical triangulations [13,14], and loop quantum gravity (LQG) [15–18]; see also [19,20] for extensive overviews), but still do not want to limit ourselves to a pure homogeneous quantum cosmology, we consider a cosmological perturbation theory with gauge-invariant variables [21,22]. We treat both the homogeneous and the inhomogeneous degrees of freedom quantum mechanically and focus particularly on the backreaction of the inhomogeneities on the homogeneous degrees of freedom.

Our work and investigations are primarily driven by the growing evidence that standard cosmology, based on general relativity and the Standard quantum Model of particle physics, needs to be extended or even rethought. Many cosmological observations point to the incompleteness of the concordance cosmological paradigm (more precisely, the ΛCDM model with cosmological perturbations and an inflaton) even though we emphasize the great successes of this model. Indirect measurements of dark energy and dark matter [23–25] or the possible tension between different measurement methods of the Hubble parameter [26–29] underline these difficulties. On the theoretical side, there already exist several approaches to overcome some of the standard model problems, both classical approaches such as theories of modified gravity [30] or cyclic universes [31], and theories of quantum cosmology such as string cosmology [32], spin-foam cosmology [33], and canonical loop quantum cosmology (LQC) [34–36]. Many of these approaches suggest that the cosmological big bang singularity should be replaced by a "big bounce," which would lead to phenomenological consequences. To test whether this prediction survives the incorporation of (quantum) fluctuations of the inhomogeneous sector is obviously of utmost importance.

As we concentrate on a quantum mechanical analysis of the problem, the most obvious proposal to answer this question consists in quantizing a classical cosmological perturbation theory. This is precisely the idea behind the

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hybrid approach to quantum cosmology, which was first applied in the context of LQC [6] but which applies as well to other theories of quantum cosmology. The approach considers the inhomogeneous sector as a quantum field theory (QFT) and the homogeneous sector as a quantum mechanical system, which are mutually in interaction. To precisely capture this interaction and to adequately estimate how it influences the effective dynamics of the homogeneous degrees of freedom is a complicated task. It has (partially) been addressed using approximations that rest on various assumptions, and we point to the dressed metric [37], the rainbow metric [38], the deformed algebra [39], and the hybrid approach [6] in this regard. Here, we employ the SAPT approach, inspired by the standard Born-Oppenheimer approximation [40], in order to study the effects of the cosmological quantum perturbations on the homogeneous quantum degrees of freedom. SAPT is a thorough extension of the Born-Oppenheimer scheme which reduces the error of the scheme up to the desired order in a perturbation theory.

In the molecular standard field of application, SAPT employs the tiny mass ratio of a molecule's constituents, i.e., the electrons and the nuclei, to define the adiabatic perturbation parameter that guides the perturbative scheme. The Born-Oppenheimer theory represents its restriction to the zeroth perturbative order. In addition to the improved accuracy, SAPT is also applicable to a much larger variety of models, in particular to constrained systems which is of importance for the cosmological case. Besides, it applies to models for which the coupling of the two system components is provided by *noncommuting* operators of the slow or homogeneous sector. Here, this is important since the Fock space vacua depend on both momentum and configuration variables of the homogeneous sector. SAPT treats this situation using Weyl quantization techniques [41,42].

In this series, we therefore advertise the space adiabatic scheme as an unbiased approach to the question of quantum cosmological perturbations and their backreaction. It is ideally suited to the problem under investigation in that it lifts the idea of classical cosmological perturbation theory to the quantum level, which allows one to employ the formalism of quantum field theory on curved spacetimes (QFT on CST) [43]. The adiabatic parameter is unsurprisingly related to the ratio of mass scales of matter and of geometry (namely the Planck mass) and, thus, is expected to be rather tiny. This is an ideal starting point for a perturbative expansion as is needed for space adiabatic *perturbation* theory.

The previous papers dealt with the many subtleties that one encounters when transferring the SAPT scheme developed for quantum systems with finitely many degrees of freedom to the field theory context. First, the space adiabatic perturbation scheme implies a formal dependence of the inhomogeneous quantum field representations on the homogeneous degrees of freedom. This raises the question whether these representations are equivalent in the field theoretical sense, a prerequisite for the applicability of SAPT [44–46]. Fortunately, since exactly the same question occurs in the hybrid scheme of quantum cosmology [47–51], this question can be answered in the affirmative once a suitable canonical transformation, exact up to second order in classical cosmological perturbation theory, has been carried out.

The second challenge for applying SAPT to the quantum field case occurs partly due to these transformations. In particular, the transformations imply that the new effective Mukhanov-Sasaki and tensor mass terms of the cosmological inhomogeneities are not positive in all regions of the homogeneous phase space. This leads to tachyonic modes. Let us, however, stress that these indefinite mass squared functions are *not due to the SAPT scheme itself or the specific transformations considered here*, but already occur in standard cosmological perturbation theory as soon as one uses gauge-invariant perturbation fields [21], e.g., the well-known Mukhanov-Sasaki variables. While such tachyonic instabilities appear frequently in the literature (see our comment in [3]), they entail a number of questions regarding for example Lorentz invariance and renormalizability [52]. In this respect, we again draw attention to Ref. [53] where a suitable set of transformations was employed to ensure positivity of the mass. However, these transformations are only known up to solving a system of semilinear partial differential equations while for SAPT, we need the explicit expressions of these functions. In our companion papers, in particular in [1], we have therefore advertised several solutions to the tachyonic issue. Our suggestions include an *ad hoc* removal of the tachyonic modes or an *ad hoc* restriction of the classical phase space to regions where the mass terms are manifestly positive. In lack of a better proposal, we adopt the second solution in the current paper for simplicity. Nevertheless, this very interesting and important problem deserves further investigation in the future.

The third challenge of cosmological SAPT becomes manifest when searching for solutions of the resulting effective Hamilton constraint or operator for the homogeneous sector. They depend on the effective mass terms which contain inverse powers of momentum *and* configuration variables of the homogeneous part. This leads to a more singular situation than one is used to in quantum cosmology, in particular in LQC where one can deal with inverse powers of the configuration variables by adopting a different quantum representation. This situation raises domain questions for the resulting effective Hamiltonian for each Fock energy band. These issues are addressed and partly solved in a more general context in [54] which we adopt for the current paper.

The final point regarding the cosmological implementation of SAPT concerns the backreaction contributions to the effective Hamiltonian which involves a sum over

inhomogeneous modes that can easily diverge. Fortunately, this does not occur up to the second adiabatic order considered here.

At the end, let us point out that the adiabatic perturbative expansion of SAPT has nothing to do with the so-called adiabatic vacua of a given order encountered in QFT on CST [55,56]. The latter define (approximate) Hadamard two-point functions in the sense of QFT on cosmological spacetimes with a fixed time dependence while in our case, the time dependence is *a priori* unspecified as we allow for backreaction between the homogeneous quantum scale factor of the cosmological background and the second order inhomogeneities in both the metric and the inflaton field.

This being said, the architecture of the remaining paper is as follows: In Sec. II, we introduce our model which is gauge-invariant cosmological perturbation theory and review the corresponding constraint analysis. These considerations follow the ideas presented in [48]. In Sec. III, we carry out the space adiabatic scheme for gauge-invariant cosmological perturbation theory. The fourth section introduces transformations that lead to a model with positive effective mass values, and we apply the space adiabatic scheme here as well. In Sec. V, we summarize and conclude. In the Appendix, we present some details of the straightforward but tedious calculations that lead to the effective Hamiltonian.

II. COSMOLOGICAL PERTURBATION THEORY AND CONSTRAINTS

A. Constraint analysis and Dirac algorithm

We consider standard cosmological perturbation theory on a four-dimensional globally hyperbolic space ime manifold $\mathcal{M} = \mathbb{R} \times \mathcal{B}$ where $\mathcal{B}$ are the three-dimensional spatial hypersurfaces. For the gravity part, we include a two-times covariant, symmetric, and nondegenerate metric field g with Lorentzian signature $(-,+,+,+)$, and for the matter part a real-valued scalar field Φ with mass $m \in \mathbb{R}^+$ as well as a cosmological constant $\Lambda \in \mathbb{R}^+$. We choose $\mathcal{B}$ to be the compact flat three-torus $\mathbb{T}^3$ with side length l in all three directions. For simplicity, we directly set $l \equiv 1$. We emphasize that the torus comprises any compact and flat manifold since they are all finitely covered by tori according to a theorem by Bieberbach [57,58]. This models a flat universe which agrees with observations as long as the side lengths of the torus are large compared to the size of the observable universe.

The space adiabatic theory as developed in [4,5] requires a Hamiltonian formulation of the problem, and consequently we adopt a $(3+1)$ split of spacetime following Arnowitt, Deser, and Misner [59] (see also [18] which gives a detailed treatment of this approach). The Cauchy surfaces Σ_t which are parametrized by a global time function t correspond to the spatial hypersurfaces $\mathbb{T}^3$. Let n be the unit normal vector field to these hypersurfaces. Furthermore, let N and $\mathcal{N}$ be the (standard) lapse and shift functions which parametrize the normal and the tangential parts of the foliation of the hypersurfaces. Then, it is possible to formulate an initial value problem for the theory, and the task of specifying constraints or equations of motion for the metric field g translates into finding the time evolution of the spatial metric $h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu$ on the hypersurfaces induced by g. The complete definition of the initial value problem requires in addition the specification of the extrinsic curvature $K_{\mu\nu} = q^\rho_\mu q^\lambda_\nu \nabla_\rho n_\lambda$ which is associated with the "time derivative" of h. ∇ is the unique torsion-free covariant derivative associated with g. After pulling back the tensor fields to $\mathbb{R} \times \mathbb{T}^3$ and denoting spatial indices on the spatial hypersurfaces with lowercase latin symbols $a, b, c, \ldots \in \{1,2,3\}$, the Einstein-Hilbert Lagrange density $\mathcal{L}_{\mathrm{EH}}$ of gravity and the scalar field Lagrange density $\mathcal{L}_\Phi$ are given by

$$\mathcal{L}_{\mathrm{EH}} = \frac{1}{2\kappa}\sqrt{|h|}N(R^{(3)} + K_{ab}K^{ab} - (K^a_a)^2 - 2\Lambda), \quad (1)$$

$$\mathcal{L}_\Phi = \frac{1}{2\lambda}\sqrt{|h|}N\left(-\frac{1}{N^2}\dot{\Phi}^2 + 2\frac{\mathcal{N}^a}{N^2}\dot{\Phi}\partial_a\Phi + \left(h^{ab} - \frac{\mathcal{N}^a\mathcal{N}^b}{N^2}\right)\partial_a\Phi\partial_b\Phi + m^2\Phi^2\right). \quad (2)$$

$\kappa = 8\pi G$ is the gravitational coupling constant, λ is the coupling constant of the scalar field, and $R^{(3)}$ is the curvature scalar associated with the three-metric h and its Levi-Civita covariant derivative D. We assume λ to have the dimension of an inverse mass squared. We stress that in usual considerations of inflation λ is set to unity for convenience.

The cosmological setting in this work suggests to consider a homogeneous and isotropic restriction of the gravitational theory up to small deviations. These symmetry reductions imply that the only remaining degrees of freedom for the homogeneous and isotropic part of the system are the zeroth order lapse function N_0 and the scale factor a, associated with the zeroth order spatial metric $h^0(t,x) = a^2(t)\tilde{h}^0(x)$ where we introduced the fixed spatial metric $\tilde{h}^0$ on the spatial hypersurfaces. Note that for the three torus $\tilde{h}^0$ is simply the standard Euclidean metric with a determinant equal to one. We will consequently omit it whenever possible. We then introduce perturbations of the spatially homogeneous and isotropic metric tensor, and for the scalar field. In this respect, it is convenient to decompose the perturbative fields into scalar, vector, and tensor parts according to their properties regarding $SO(3)$ transformations (in the limit of an infinite compactification scale). This is reasonable because the respective equations of motion decouple. Note that the procedure of introducing perturbative fields on a homogeneous and isotropic

background introduces a gauge freedom for the perturbations since the choice of coordinates is *a priori* arbitrary. A detailed analysis of cosmological perturbation theory within the Hamiltonian framework for closed Friedman-Lemaître-Robertson-Walker (FLRW) universes can be found in [60]. There, however, the gauge freedom of the perturbations was fixed by choosing one particular gauge. We therefore refer to [48], at least regarding the scalar part of the perturbations, where the authors use gauge-invariant Mukhanov-Sasaki perturbations. For the tensor perturbations, we point to [61]. Similar to the definitions in [48,61], we define the perturbed lapse, shift, spatial metric, and matter scalar field, respectively, as

$$N(t,x) =: N_0(t) + a^3(t)\eta(t,x), \tag{3}$$

$$\mathcal{N}_a(t,x) =: a^2(t)D_a k(t,x) + a^2(t)\epsilon_a^{bc}D_b k_c(t,x), \tag{4}$$

$$\begin{aligned} h_{ab}(t,x) =: a^2(t)\Big[&(1+2\alpha(t,x))\tilde{h}^0_{ab}(x) \\ &+ 6\left(D_aD_b - \frac{1}{3}\tilde{h}^0_{ab}(x)\Delta\right)\beta(t,x) \\ &+ 4\sqrt{3}D_{(a}V_{b)}(t,x) + 2\sqrt{6}t_{ab}(t,x)\Big], \end{aligned} \tag{5}$$

$$\Phi(t,x) =: \phi(t) + \varphi(t,x), \tag{6}$$

where $\Delta := D_aD^a$ denotes the Laplace-Beltrami operator on $\mathbb{T}^3$. The homogeneous and isotropic degrees of freedom are hence (N_0, a, ϕ) while the inhomogeneous fields are subdivided into the scalar perturbations $(\eta, k, \alpha, \beta, \varphi)$, the vector degrees of freedom v_a and k_a, and the tensor field perturbations t_{ab}. For notational reasons, we introduce the fields $\check{k} := \Delta k$ and $\check{k}_a := \epsilon_a^{bc}D_b k_c$ as new degrees of freedom associated with the shift function. In contrast to the proceeding in [48,61], we stick to a spacetime representation of the perturbative fields instead of choosing a particular Fourier mode decomposition, at least for the time being.

The next step toward a thorough constraint analysis of the system consists of inserting the perturbed variables of the definitions (3), (4), (5), and (6) into the Lagrange density (1), (2), and then to expand the Lagrangian and the action functional S up to second order in the perturbations. As the three-torus does not have a boundary, total divergences vanish. The resulting action depends neither on the velocities of the lapse variables N_0 and η nor on the velocities of the shift variables $\check{k}$ and $\check{k}_a$. This implies that lapse and shift are Lagrange multipliers and will hence be associated with primary constraint equations in the Hamiltonian formalism. In order to pass over to the Hamiltonian picture, we perform a Legendre transformation in the lines of [48,60]. Thereby, we define the conjugate momenta (P_a, P_ϕ) for the homogeneous and isotropic degrees of freedom (a, ϕ) in the standard manner by means of the Lagrange function $L = \int \mathrm{d}x\mathcal{L}$,

$$P_a := \frac{\partial L}{\partial \dot{a}} = -\frac{6}{\kappa N}a\dot{a}, \qquad P_\phi := \frac{\partial L}{\partial \dot{\phi}} = \frac{a^3}{\lambda N}\dot{\phi}. \tag{7}$$

We denote the corresponding phase space by Γ_{hom}. Furthermore, the perturbation fields α, β, φ, v_a, and t_{ab} together with their conjugate momenta π_α, π_β, π_φ, π_v^a, and π_t^{ab} span the perturbative phase space Γ_{pert}. The momenta are defined in the standard way according to

$$\pi_\theta := \frac{\partial \mathcal{L}}{\partial \dot{\theta}}, \tag{8}$$

for any field $\theta \in \{\alpha, \beta, \varphi, v_a, t_{ab}\}$. On the other hand, the variables N_0, η, $\check{k}$, and $\check{k}_a$ induce the lapse and shift primary constraints $\Pi_0^{N_0}$, Π_1^η, $\Pi_1^{\check{k}}$, and $\Pi_1^{\check{k}_a,b}$ because the Lagrangian does not depend on any of the velocities of these variables. The Legendre transformation yields a Hamiltonian density of the form

$$\begin{aligned} \mathcal{H} = N_0[\mathcal{H}_0 + \mathcal{H}_2^{\mathrm{s}} + \mathcal{H}_2^v + \mathcal{H}_2^t] + \eta\cdot\mathcal{H}_1^\eta + \check{k}_a\cdot\mathcal{H}_1^{\check{k}_a,a} + \check{k}\cdot\mathcal{H}_1^{\check{k}} \\ + \lambda_{N_0}\cdot\Pi_0^{N_0} + \lambda_\eta\cdot\Pi_1^\eta + \lambda_{\check{k}}\cdot\Pi_1^{\check{k}} + \lambda_{\check{k}_a,b}\cdot\Pi_1^{\check{k}_a,b}. \end{aligned} \tag{9}$$

Here, $\mathcal{H}_0$ denotes the zeroth order Hamiltonian contribution associated with the completely homogeneous and isotropic model. The contributions $\mathcal{H}_2^{\mathrm{s}}$, $\mathcal{H}_2^v$, and $\mathcal{H}_2^t$ are of second order in the perturbations and contain only scalar, vector, and tensor variables, respectively. The functions $\mathcal{H}_1^\eta$, $\mathcal{H}_1^{\check{k}_a,a}$, and $\mathcal{H}_1^{\check{k}}$ represent first order contributions which factorize with the respective lapse and shift variables. The second line only lists the primary constraints associated with lapse and shift and their Lagrange multipliers λ_{N_0}, λ_η, $\lambda_{\check{k}}$, and $\lambda_{\check{k}_a,b}$.

Before we give the concrete representation of the Hamiltonian (9), we carry out a Dirac analysis to filter out the relevant terms of $\mathcal{H}$. As a matter of fact, the system is completely constrained such that it is indeed reasonable to perform a Dirac analysis. Thereby, we encounter several difficulties: First, the perturbation variables that we introduced are not all gauge invariant. Therefore, a canonical transformation to gauge-invariant variables is necessary in order to have a covariant perturbation theory. Indeed, it is straightforward to introduce the gauge-invariant Mukhanov-Sasaki variable ϑ in the scalar sector of the perturbations; see for example [21,22]

$$\vartheta := af + \frac{6\lambda P_\phi}{\kappa P_a}(\alpha - \Delta\beta). \tag{10}$$

Thereby, we perform a transformation for the perturbations only but which depends on the homogeneous degrees of

freedom. In order to preserve the canonical structure of the system, it is mandatory to find a suitable transformation for the homogeneous and isotropic variables, too. This appears to be a cumbersome mission. However, the authors of [48] have shown that it is possible to find a transformation for the homogeneous and isotropic degrees of freedom which preserves the canonical structure of the system up to second order in the cosmological perturbations.

The second difficulty regarding the Dirac algorithm concerns the closure of the constraint algebra. In general, the algorithm might entail a large number of constraints which are not well manageable. The idea, put forward in [48,61] which we will also apply in this work, is to use some of the secondary constraints of the Dirac algorithm as the canonical variables themselves. Thereby, the Dirac algorithm becomes partly trivial just by implementing the first set of secondary constraints. This will be demonstrated in the sequel. In summary, the aim of the following procedure is then threefold: First, we introduce gauge-invariant variables for the perturbations. Second, we aim at keeping the canonical structure of the theory, at least up to second order in the cosmological perturbations. Therefore, we review the Dirac algorithm for constrained systems and implement additional transformations for the homogeneous and isotropic degrees of freedom. In particular, we modify the homogeneous variables by adding second order contributions of the perturbations. Third, we wish to construct a theory whose dynamics will be unitarily implementable at the quantum level. Therefore, we consider further canonical transformations with respect to the perturbations. Their effects on the homogeneous variables will be taken into account accordingly.

Following [48,61], the formalism proceeds as follows: We first consider the homogeneous and isotropic degrees of freedom as nondynamical background variables. This offers the possibility to introduce perturbation variables which build a canonical set with respect to the dynamical, perturbative system only. We start with the canonical pair of the tensor perturbations (t_{ab}, π_t^{ab}) which is already gauge invariant. However, we aim at obtaining classical perturbation variables whose dynamics is unitarily implementable in the quantum realm. As shown for example in [47,50,51], this simply amounts to eliminating contributions in the Hamiltonian which couple the perturbation variables with their respective momenta. In this way, the final Hamiltonian at second order will only consist of terms proportional to squares of the perturbation variables or squares of the perturbation momenta. In other words, after a Fourier transformation the Hamiltonian has the form of a sum of harmonic oscillators with masses and frequencies that possibly depend on the homogeneous and isotropic degrees of freedom. Indeed, these transformations guarantee the unitarity of the perturbation's quantum dynamics when considered in a semiclassical framework of QFT on CST. We employ the transformations from [61] for the tensor perturbations and thereby transform the homogeneous degrees of freedom accordingly by adding second order field contributions. We denote the shifted, new homogeneous variables by $(\check{a}, \check{P}_a, \check{\phi}, \check{P}_\phi)$. The transformations yield additional terms in the Hamiltonian which are of second order in the tensor perturbations. We absorb these terms in $\mathcal{H}_2^t$ and denote the new tensor Hamiltonian as $\check{\mathcal{H}}_2^t$. Furthermore, the transformations result in a shift of the lapse function by second order contributions which we take into account by a function denoted by $\check{N}_2$.

Regarding the vector perturbations, we can identify the constraints $\mathcal{H}_1^{\check{k}_d,a}$ and their conjugate variables $C_{1,a}^{\check{k}_d} = 2\sqrt{3}v_a$ as canonical pairs. The transformation for these perturbation variables entails a transformation for the homogeneous degrees of freedom in order to keep the (almost) canonical structure, just as for the tensor perturbations. The new variables, which also include the transformations due to the tensor perturbations, are denoted by $(\grave{a}, \grave{P}_a, \grave{\phi}, \grave{P}_\phi)$. The transformations result in a new second order vectorial part of the Hamiltonian, $\grave{\mathcal{H}}_2^v$, which is proportional to the constraint $\mathcal{H}_1^{\check{k}_d,a}$ itself. Note that we also express the linear constraint $\mathcal{H}_1^{\check{k}_d,a}$ in terms of the new variables. However, the form of the constraint does not change since we cut after the second perturbative order and the new homogeneous variables only differ by contributions in the second order. Thus, if we demand that $\mathcal{H}_1^{\check{k}_d,a}$ vanishes as a constraint, this implies that $\grave{\mathcal{H}}_2^v$ vanishes automatically. We can therefore omit the further analysis of the vector perturbations.

In the scalar sector, we employ the Mukhanov-Sasaki scalar field ϑ as introduced above. As suggested in [48], it is clever to additionally consider the first order constraints $\mathcal{H}_1^\eta$ and $\mathcal{H}_1^{\check{k}}$ as new perturbation variables. Since these constraints do not commute with respect to the perturbation Poisson brackets, we shift $\mathcal{H}_1^\eta$ by a linear term in the perturbations and we denote the new constraint variable by $\bar{\mathcal{H}}_1^\eta$. The latter Poisson commutes with $\mathcal{H}_1^{\check{k}}$, if for the time being we only consider the perturbations as dynamical degrees of freedom. This procedure entails another shifting of the lapse function which yields the new lapse function, $\bar{N}_2$ from $\check{N}_2$. In the next step, we construct the conjugate variables with respect to the *inhomogeneous* Poisson brackets, denoting them by π_ϑ, C_1^η, and $C_1^{\check{k}}$. The new canonical pairs in the scalar sector of the perturbations are, thus, $(\vartheta, \pi_\vartheta)$, $(C_1^\eta, \bar{\mathcal{H}}_1^\eta)$, and $(C_1^{\check{k}}, \mathcal{H}_1^{\check{k}})$. Finally, we complete the transformation in the homogeneous sector by adding second order contributions to the initial homogeneous canonical pairs. The procedure for obtaining the correct contributions can be found in [48]. It yields a new set of variables $(\tilde{a}, \tilde{P}_a, \tilde{\phi}, \tilde{P}_\phi)$ in the homogeneous sector. The implementation of the transformations yields new

contributions to $\mathcal{H}$: Some of them include only the Mukhanov-Sasaki canonical variables, and we correspondingly absorb them into a new second order scalar Hamiltonian $\tilde{\mathcal{H}}_2^s$; another contribution is proportional to the zeroth order Hamiltonian $\mathcal{H}_0$ such that it is possible to absorb them into $\bar{N}_2$ giving $\check{N}_2$. In addition, the transformations result in new second order contributions which are proportional to the linear constraints $\bar{\mathcal{H}}_1^\eta$ and $\mathcal{H}_1^{\check{k}}$. We denote these contributions as G_1 and K_1, respectively. In total, the transformations result in the following Hamiltonian density:

$$\begin{aligned}\tilde{\mathcal{H}} &= (N_0 + \check{N}_2)\cdot[\mathcal{H}_0 + \tilde{\mathcal{H}}_2^s + \grave{\mathcal{H}}_2^v + \check{\mathcal{H}}_2^t] \\ &\quad + (\eta + G_1)\cdot\bar{\mathcal{H}}_1^\eta + (\tilde{k} + K_1)\cdot\mathcal{H}_1^{\check{k}} + \check{k}_a\cdot\mathcal{H}_1^{\check{k}_d,a} \\ &\quad + \lambda_{N_0}\cdot\Pi_0^{N_0} + \lambda_\eta\cdot\Pi_1^\eta + \lambda_{\check{k}}\cdot\Pi_1^{\check{k}} + \lambda_{\check{k}_b,a}\cdot\Pi_1^{\check{k}_b,a}. \quad (11)\end{aligned}$$

We emphasize that the constraint $\tilde{\mathcal{H}}$ is to be expressed in terms of the new homogeneous variables $(\tilde{a}, \tilde{P}_a, \tilde{\phi}, \tilde{P}_\phi)$, which finally amounts to simply replacing nondashed variables by the dashed ones as we truncate after the second order in perturbations. The second line in Eq. (11) accounts for the set of primary constraints $(\Pi_0^{N_0}, \Pi_1^\eta, \Pi_1^{\check{k}}, \Pi_1^{\check{k}_b,a})$ with their respective Lagrange multipliers, $(\lambda_{N_0}, \lambda_\eta, \lambda_{\check{k}}, \lambda_{\check{k}_b,a})$. These primary constraints already appeared in Eq. (9) and have remained unchanged under the preceding transformations. The system restricts to the submanifold of the phase space defined by the primary constraints,

$$\Pi_0^{N_0} = 0, \qquad \Pi_1^\eta = 0, \qquad \Pi_1^{\check{k}} = 0, \qquad \Pi_1^{\check{k}_b,a} = 0. \quad (12)$$

Consequently, the associated Lagrange multipliers can be chosen arbitrarily. In a second step, consistency of the dynamics requires that the primary constraints remain zero under the evolution generated by the full Hamilton constraint $\tilde{\mathcal{H}}$. This requirement gives rise to the secondary constraints,

$$\{\tilde{\mathcal{H}}, \Pi_0^{N_0}\} = \mathcal{H}_0 + \tilde{\mathcal{H}}_2^s + \grave{\mathcal{H}}_2^v + \check{\mathcal{H}}_2^t \approx 0, \quad (13)$$

$$\{\tilde{\mathcal{H}}, \Pi_1^\eta\} = \bar{\mathcal{H}}_1^\eta \approx 0, \quad (14)$$

$$\{\tilde{\mathcal{H}}, \Pi_1^{\check{k}}\} = \mathcal{H}_1^{\check{k}} \approx 0, \quad (15)$$

$$\{\tilde{\mathcal{H}}, \Pi_1^{\check{k}_b,a}\} = \mathcal{H}_1^{\check{k}_b,a} \approx 0, \quad (16)$$

where "≈0" means that the expression on the left-hand side must vanish at least weakly, i.e., on the primary constraint surface. Note that now the Poisson brackets include the dynamics with respect to *all* canonical pairs of the transformed system, both the homogeneous and the inhomogeneous ones. Indeed, the formalism allows us to compute the dynamics for the full system in the standard Hamiltonian framework. The next step consists in checking whether the secondary constraints in Eqs. (13)–(16) are preserved under the dynamics of $\tilde{\mathcal{H}}$, or if they entail further secondary constraints. The computations are in fact trivial since the preceding transformations imply that the first order constraints $(\bar{\mathcal{H}}_1^\eta, \mathcal{H}_1^{\check{k}}, \mathcal{H}_1^{\check{k}_d,a})$ are canonical variables, and hence commute with all other variables except with their conjugate variables, $(C_1^\eta, C_1^{\check{k}}, C_1^{\check{k}_d,a})$. Indeed, C_1^η appears in $\tilde{\mathcal{H}}$ within the first order functions G_1 and K_1 and, thus, entails nonvanishing Poisson brackets with $\bar{\mathcal{H}}_1^\eta$. Since these Poisson brackets enter, however, with an additional constraint factor, they vanish at least weakly, namely

$$\{\tilde{\mathcal{H}}, \mathcal{H}_0 + \tilde{\mathcal{H}}_2^s + \grave{\mathcal{H}}_2^v + \check{\mathcal{H}}_2^t\} = 0, \quad (17)$$

$$\{\tilde{\mathcal{H}}, \bar{\mathcal{H}}_1^\eta\} = \{G_1, \bar{\mathcal{H}}_1^\eta\}\bar{\mathcal{H}}_1^\eta + \{K_1, \bar{\mathcal{H}}_1^\eta\}\mathcal{H}_1^{\check{k}} \approx 0, \quad (18)$$

$$\{\tilde{\mathcal{H}}, \mathcal{H}_1^{\check{k}}\} = \{G_1, \mathcal{H}_1^{\check{k}}\}\bar{\mathcal{H}}_1^\eta + \{K_1, \mathcal{H}_1^{\check{k}}\}\mathcal{H}_1^{\check{k}} = 0. \quad (19)$$

In summary, the constraint algebra closes and we are able to solve the dynamics of the system. Therefore, the primary constraints (12), as well as the secondary constraints,

$$\begin{aligned}&\bar{\mathcal{H}}_1^\eta = 0, \qquad \mathcal{H}_1^{\check{k}} = 0, \qquad \mathcal{H}_1^{\check{k}_b,a} = 0, \\ &\mathcal{H}_0 + \tilde{\mathcal{H}}_2^s + \grave{\mathcal{H}}_2^v + \check{\mathcal{H}}_2^t = 0, \quad (20)\end{aligned}$$

must be satisfied on the constraint surface. Since $\bar{\mathcal{H}}_1^\eta$, $\mathcal{H}_1^{\check{k}}$, and $\mathcal{H}_1^{\check{k}_b,a}$ were simply defined as canonical momenta, it is not necessary to analyze these constraints further. We recall that the second order vector constraint $\grave{\mathcal{H}}_2^v$ is zero whenever $\mathcal{H}_1^{\check{k}_b,a} = 0$ holds true. Hence, the only nontrivial constraint of the cosmological system amounts to be

$$\mathcal{C} \coloneqq \mathcal{H}_0 + \tilde{\mathcal{H}}_2^s + \check{\mathcal{H}}_2^t = 0. \quad (21)$$

The total constraint $C = \int \mathrm{d}x\mathcal{C}$ splits into the three parts

$$H_0 \coloneqq -\kappa\frac{\tilde{P}_a^2}{12\tilde{a}} + \frac{\Lambda}{\kappa}\tilde{a}^3 + \frac{\lambda\tilde{P}_\phi^2}{2\tilde{a}^3} + \frac{1}{2\lambda}m^2\tilde{a}^3\tilde{\phi}^2, \quad (22)$$

$$\tilde{H}_2^s \coloneqq \frac{1}{2\tilde{a}}\int_{\mathbb{T}^3}\mathrm{d}x\left(\lambda\pi_\vartheta^2 + \vartheta\left(-\frac{\Delta}{\lambda} + M_{\mathrm{MS}}(\tilde{a}, \tilde{P}_a, \tilde{\phi}, \tilde{P}_\phi)^2\right)\vartheta\right), \quad (23)$$

$$\check{H}_2^t \coloneqq \frac{1}{2\tilde{a}}\int_{\mathbb{T}^3}\mathrm{d}x\left(\frac{\kappa\pi_t^{ab}\pi_{ab}^t}{6} + t^{ab}\left(-\frac{3\Delta}{\kappa} + M_{\mathrm{T}}(\tilde{a}, \tilde{P}_a, \tilde{\phi})^2\right)t_{ab}\right), \quad (24)$$

where we recall that $(\vartheta, \pi_\vartheta, t_{ab}, \pi_t^{ab})$ are inhomogeneous and thus x-dependent fields. We defined the Mukhanov-Sasaki mass function $M_{\mathrm{MS}}(\tilde{a}, \tilde{P}_a, \tilde{\phi}, \tilde{P}_\phi)$ and the tensor mass function $M_{\mathrm{T}}(\tilde{a}, \tilde{P}_a, \tilde{\phi})$ according to

$$M_{\mathrm{MS}}^2 := -\frac{\kappa^2\tilde{P}_a^2}{18\lambda\tilde{a}^2} + \frac{7\kappa\tilde{P}_\phi^2}{2\tilde{a}^4} - 12m^2\frac{\tilde{a}\tilde{\phi}\tilde{P}_\phi}{\lambda\tilde{P}_a} - 18\frac{\lambda\tilde{P}_\phi^4}{\tilde{a}^6\tilde{P}_a^2} + \frac{m^2}{\lambda}\tilde{a}^2,$$
$$M_{\mathrm{T}}^2 := \frac{\kappa\tilde{P}_a^2}{6\tilde{a}^2} - 3\frac{m^2}{\lambda}\tilde{a}^2\tilde{\phi}^2 - 6\frac{\Lambda}{\lambda}\tilde{a}^2. \tag{25}$$

The total Hamiltonian $C = H_0 + \tilde{H}_2^s + \check{H}_2^t$ is the object of interest in this work, and we will prepare it accordingly for the application to the space adiabatic scheme.

B. The Hamilton constraint

First, we recall that the system variables consist, on the one hand, of the homogeneous and isotropic canonical pairs $(\tilde{a}, \tilde{P}_a)$ and $(\tilde{\phi}, \tilde{P}_\phi)$. These are associated with the standard cosmological scale factor a and the homogeneous and isotropic parts of the scalar matter field ϕ but have been shifted by second order contributions in the cosmological perturbations in order to maintain the (almost) canonical structure of the system. In order to make the space adiabatic scheme work at the technical level, we rescale several variables and we define the dimensionless parameter ε according to

$$\varepsilon^2 := \frac{\kappa}{\lambda}. \tag{26}$$

To see that ε^2 is indeed tiny recall that the reduced Planck mass is given by $M_{\mathrm{Pl}} = \sqrt{\hbar c/\kappa} \approx 2.43 \times 10^{18}\ \mathrm{GeV}/c^2$, while the mass of the heaviest known Standard Model particle (the Higgs boson) is $M_{\mathrm{H}} \approx 125.09\ \mathrm{GeV}/c^2 \ll M_{\mathrm{Pl}}$. Assuming that $\lambda^{-1/2}$ does not exceed M_{H} substantially, we have indeed that $\varepsilon^2 \sim 10^{-32}$. Note that we implicitly choose the fields ϕ and φ to be dimensionless. In this way, we do not need to introduce additional mass scales into more general than quadratic inflaton potentials. The scheme suggests to rescale the homogeneous degrees of freedom according to

$$\check{p}_a := \varepsilon^2\tilde{P}_a, \qquad \check{p}_\phi := \varepsilon\tilde{P}_\phi, \tag{27}$$

as well as the Mukhanov-Sasaki field variables $(\vartheta, \pi_\vartheta)$ and the tensor field variables (t_{ab}, π_t^{ab}) as

$$\breve{\vartheta} := \frac{\vartheta}{\varepsilon}, \quad \breve{\pi}_\vartheta := \varepsilon\pi_\vartheta \ \text{ and } \ \breve{t}_{ab} := \frac{t_{ab}}{\varepsilon^2}, \quad \breve{\pi}_t^{ab} := \varepsilon^2\pi_t^{ab}. \tag{28}$$

We directly relabel the rescaled variables by removing the breves such that the notation remains as simple as possible. Besides, we omit the dashes on $\tilde{a}$ and $\tilde{\phi}$. Because the function C is constrained to vanish, it is admissible to multiply it by a global factor of ε^2. This gives the final classical Hamilton constraint $C = H_0 + \tilde{H}_2^s + \check{H}_2^t = 0$ where now any of the terms are rescaled by a factor of ε^2 such that

$$H_0 = -\frac{p_a^2}{12a} + \frac{p_\phi^2}{2a^3} + \frac{1}{2}\varepsilon^2 m^2 a^3\phi^2 + \Lambda a^3, \tag{29}$$

$$\tilde{H}_2^s = \frac{1}{2a}\int_{\mathbb{T}^3} \mathrm{d}x(\pi_\vartheta^2 + \vartheta\varepsilon^4(-\Delta + M_{\mathrm{MS}}^2)\vartheta), \tag{30}$$

$$\check{H}_2^t = \frac{1}{2a}\int_{\mathbb{T}^3} \mathrm{d}x\left(\frac{\pi_t^{ab}\pi_{ab}^t}{6} + t^{ab}\varepsilon^4(-3\Delta + (\varepsilon M_{\mathrm{T}})^2)t_{ab}\right), \tag{31}$$

for which we employed the corresponding Mukhanov-Sasaki and tensor mass squared functions

$$M_{\mathrm{MS}}^2 = -\frac{p_a^2}{18a^2} + \frac{7p_\phi^2}{2a^4} - 12\varepsilon m^2\frac{a\phi p_\phi}{p_a} - 18\frac{p_\phi^4}{a^6p_a^2} + m^2a^2, \tag{32}$$

$$(\varepsilon M_{\mathrm{T}})^2 = \frac{p_a^2}{6a^2} - 3\varepsilon^2m^2a^2\phi^2 - 6\Lambda a^2. \tag{33}$$

Note that the transformations for the perturbation fields (28) are canonical while the canonical structure of the homogeneous degrees of freedom changes due to the rescaling in (27). This becomes evident when considering the canonical quantum commutation relations in the following. Indeed, SAPT considers the whole system as a quantum system—it does not rely on any semiclassical approximation.

Therefore, we employ a standard Schrödinger representation in the homogeneous sector of the quantum theory, and we introduce hats for indicating quantum operators. We denote the Hilbert spaces of the gravitational subsystem associated with the scale factor as $\mathcal{H}_a = L^2(\mathbb{R}^+, \mathrm{d}a)$ and the homogeneous scalar matter subsystem $\mathcal{H}_\phi = L^2(\mathbb{R}, \mathrm{d}\phi)$. The total homogeneous Hilbert space is given as the topological tensor product $\mathcal{H}_{\mathrm{hom}} = \mathcal{H}_a \otimes \mathcal{H}_\phi$. The operators for the homogeneous sector $(\hat{a}, \hat{p}_a, \hat{\phi}, \hat{p}_\phi)$ are associated with the standard multiplication and derivative operators in the Schrödinger position representation on the respective dense domains. Note that due to the rescaling with ε, the momentum operators always enter with an additional factor ε^2 or ε, respectively. Their Weyl elements satisfy the Weyl algebra relations which lead to the formal quantum commutation relations,

$$[\hat{a}, \hat{p}_a]_a = i\varepsilon^2\hat{1}_a, \qquad [\hat{\phi}, \hat{p}_\phi]_\phi = i\varepsilon\hat{1}_\phi. \tag{34}$$

The operators $\hat{1}_a$ and $\hat{1}_\phi$ denote the unity operators in the respective quantum algebras. The application of SAPT to our cosmological model considers the homogeneous and

isotropic degrees of freedom as the ones whose canonical structure becomes rescaled by a very small parameter. Indeed, we have shown in [1] that the homogeneous variables can be understood as the slow and heavy center of mass modes of the system.

The fast sector of the model is thus associated with the cosmological inhomogeneities, i.e., the Mukhanov-Sasaki and tensor perturbations. We choose bold characters to indicate quantum operators of the inhomogeneous system just as in the preceding papers of the series. In particular, the basic quantum fields of the theory are given for any fixed time $t \in \mathbb{R}$ by the operator-valued distributions $(\boldsymbol{\vartheta}, \boldsymbol{\pi}_\vartheta, \boldsymbol{t}_{ab}, \boldsymbol{\pi}_t^{ab})$ on the spatial manifold $\mathbb{T}^3$. We denote the Hilbert space of the Mukhanov-Sasaki quantum system by $\mathcal{H}_{\mathrm{MS}}$ and the Hilbert space of the tensor perturbations by $\mathcal{H}_{\mathrm{T}}$, and the total Hilbert space of the inhomogeneities arises naturally as the tensor product of the two latter $\mathcal{H}_{\mathrm{pert}} = \mathcal{H}_{\mathrm{MS}} \otimes \mathcal{H}_{\mathrm{T}}$. We employ the standard canonical commutation relations for the perturbation fields and therefore introduce two contravariant test tensor fields $f(x)$ and $F_{ab}(x)$ of rank 0 and 2, respectively, as well as two covariant test tensor fields $j(x)$ and $J^{ab}(x)$ of rank 0 and 2, respectively. The quantum commutation relations consequently have the form

$$[j(\boldsymbol{\vartheta}), \boldsymbol{\pi}_\vartheta(f)]_{\mathrm{MS}} = i\langle f, j\rangle \mathbf{1}_{\mathrm{MS}},$$
$$[J(\boldsymbol{t}), \boldsymbol{\pi}_t(F)]_{\mathrm{T}} = i\langle F^{ab}, J_{ab}\rangle \mathbf{1}_{\mathrm{t}},$$

where $\langle \cdot, \cdot \rangle$ denotes the standard L^2-inner product on the three-torus. SAPT makes explicit use of the Hilbert space representation for the perturbative fields as employed here. However, it uses a different representation for the homogeneous degrees of freedom, as explained in [5] but also in [1,2] in more detail. In particular, the homogeneous sector is subject to a phase space or deformation quantization [62–65] which represents quantum operators as scalar functions on phase space. In this representation, the commuting pointwise product of functions from the classical theory transforms into a noncommuting product of the phase space functions which has here the form of a power series expansion in the perturbation parameter ε. The product is well-known as Moyal or star product in the theory of phase space quantization [66,67].

We emphasize that this quantization scheme is physically equivalent to the standard Hilbert space representation but it allows for a perturbative treatment of the coupled quantum systems that we have in mind. The relation between the phase space scheme and the Hilbert space approach is established by associating the phase space functions of the first approach with integral kernels of operators in the Hilbert space picture. In the following, we explicitly employ quantum operators on Hilbert spaces with respect to the inhomogeneous fields while using the phase space picture of the homogeneous sector, thus treating the homogeneous variables *formally* as real-valued functions on the homogeneous phase space. This leads us to introduce operator-valued functions on the homogeneous phase space Γ_{hom}, also denoted as operator-valued "symbol functions," and we generically write for the class of such functions $S(\Gamma_{\mathrm{hom}}, \mathcal{L}(\mathcal{H}_{\mathrm{pert}}))$. The theory of pseudodifferential calculus (see, e.g., [68]) addresses the question about which of these symbol functions leads to well-defined operators on different function spaces.

Therefore, let us introduce the relevant operator-valued functions here. For our purposes, it is useful to perform a transformation to annihilation and creation operators. Therefore, let us consider the one-particle Hilbert space $\mathcal{H}_{\mathbb{T}^3} = L^2(\mathbb{T}^3, \mathrm{d}x)$ on the compact three-torus. A suitable choice of basis is the set of functions $\{f_k(x) = \exp(ikx)\}_k$ labeled by the discrete vectors $k \in \mathbb{k} := 2\pi\mathbb{Z}^3\backslash\{0\}$. The Hilbert spaces of the perturbative quantum field theories are then given as the symmetric Fock spaces $\mathcal{F}_{\mathrm{s}}(\mathcal{H}_{\mathbb{T}^3})$ associated with the one-particle Hilbert space. More precisely, the total perturbative Hilbert space comprises the Mukhanov-Sasaki real scalar field Fock space, $\mathcal{F}_{s,\mathrm{MS}}$, as well as two Fock spaces associated with the tensor degrees of freedom. Indeed, the tensor field carries only two independent degrees of freedom corresponding to the two polarizations of the tensor modes. These will be labeled by the index $\tau = \{+, -\}$, and we write for the Fock spaces $\mathcal{F}_{\mathrm{s,T},\pm}$. The total Hilbert space is given as the topological tensor product

$$\mathcal{H}_{\mathrm{pert}} = \mathcal{F}_{\mathrm{s,MS}}(\mathcal{H}_{\mathbb{T}^3}) \bigotimes_{\tau=\{+,-\}} \mathcal{F}_{s,\mathrm{T},\tau}(\mathcal{H}_{\mathbb{T}^3}). \tag{35}$$

The relevant annihilation and creation operators act by destroying and, respectively, generating one-particle states $f \in \mathcal{H}_{\mathbb{T}^3}$ on Fock space. Let us therefore define the one-particle frequency operators for the Mukhanov-Sasaki and the tensor systems by

$$\omega_{\mathrm{MS}} := \varepsilon^2\sqrt{-\Delta + M_{\mathrm{MS}}^2}, \qquad \omega_{\mathrm{T}} := \varepsilon^2\sqrt{-18\Delta + 6(\varepsilon M_{\mathrm{T}})^2}. \tag{36}$$

Note that both operators depend on the homogeneous degrees of freedom as they contain the mass functions $M_{\mathrm{MS}}(a, p_a, \phi, p_\phi)$ and $M_{\mathrm{T}}(a, p_a, \phi)$. To define annihilation and creation operators of the Mukhanov-Sasaki system, we define (a, p_a, ϕ, p_ϕ)-dependent representations $\pi_{(a,p_a,\phi,p_\phi)} : \mathcal{A}_Q \to \mathcal{L}(\mathcal{F}_{s,\mathrm{MS}})$ that maps the field Weyl algebra to the space of linear operators on the Mukhanov-Sasaki Fock space. For some one-particle state $f \in \mathcal{H}_{\mathbb{T}^3}$ we obtain the following expression:

$$\boldsymbol{b}((a, p_a, \phi, p_\phi), f) := \frac{1}{\sqrt{2}}\pi_{(a,p_a,\phi,p_\phi)}[(\sqrt{\omega_{\mathrm{MS}}}\boldsymbol{\vartheta})(f) - i(\sqrt{\omega_{\mathrm{MS}}}^{-1}\boldsymbol{\pi}_\vartheta)(f)]. \tag{37}$$

The creation operator $\boldsymbol{b}^*(f)$ derives from $\boldsymbol{b}(f)$ by taking its adjoint. Likewise, one defines annihilation and creation operators $\boldsymbol{d}_\pm(f)$ and $\boldsymbol{d}^*_\pm(f)$ for the two tensor modes by replacing ω_{MS} by ω_{T} and by replacing the fields $(\boldsymbol{\vartheta}, \boldsymbol{\pi}_\vartheta)$ by the two pairs of tensorial fields which we denote by $(\boldsymbol{t}_\pm, \boldsymbol{\pi}_{t,\pm})$.

For fixed homogeneous variables (a, p_a, ϕ, p_ϕ), the canonical quantum commutation relations for the Mukhanov-Sasaki field evaluate to $[\boldsymbol{b}(f_1), \boldsymbol{b}^*(f_2)]_{\mathrm{MS}} = \mathbf{1}_{\mathrm{MS}}\langle f_1, f_2\rangle$ where $f_1, f_2 \in \mathcal{H}_{\mathbb{T}^3}$. Again, the commutation relations for the tensor part arise completely analogously. For our purposes, it is simplest to pass to a mode representation, and in the following we refer to the annihilation and creation operators of a mode k for the Mukhanov-Sasaki system by $\boldsymbol{b}_k$ and $\boldsymbol{b}^*_k$. For the tensor modes, we define the set of vectors $K \in \mathbb{K} \coloneqq \{\mathbb{k}, \tau\}$ to denote the annihilation and creation operators by $\boldsymbol{d}_K$ and $\boldsymbol{d}^*_K$. The commutation relations have the form

$$[\boldsymbol{b}_k, \boldsymbol{b}^*_{k'}]_{\mathrm{MS}} = \delta_{k,k'}\mathbf{1}_{\mathrm{MS}}, \qquad [\boldsymbol{d}_K, \boldsymbol{d}^*_{K'}]_{\mathrm{T}} = \delta_{K,K'}\mathbf{1}_{\mathrm{T}}, \tag{38}$$

and the δ's are Kronecker deltas. To evaluate the frequency operators ω with respect to the mode functions $f_k(x)$, we note that the f_k's are eigenfunctions of the Laplace-Beltrami operator, namely $(\Delta f_k)(x) = -k^2 f_k(x)$. Therefore, it is possible to label the frequency operators accordingly by $\omega_{\mathrm{MS},k}$ and $\omega_{\mathrm{T},K}$ when evaluated on f_k. It is then straightforward to express the Hamilton constraint symbol function by means of the creation and annihilation operators and the associated frequency functions. Therefore, recall that SAPT employs a phase space quantization scheme for the homogeneous sector such that the homogeneous variables appear as real functions on the homogeneous phase space while the perturbations are subject to the standard operator quantization. Using the standard techniques of QFT on CST, the normal-ordered Hamilton constraint $\boldsymbol{C} \in S(\Gamma_{\mathrm{hom}}, \mathcal{L}(\mathcal{H}_{\mathrm{pert}}))$ arising from the classical Hamilton constraint $C = H_0 + \tilde{H}^s_2 + \check{H}^t_2$ with the specifications in (29)—(31) is given by

$$\begin{aligned}\boldsymbol{C} = &\left(-\frac{p_a^2}{12a} + \frac{p_\phi^2}{2a^3} + \frac{1}{2}\varepsilon^2 m^2 a^3 \phi^2 + \Lambda a^3\right)\mathbf{1}_{\mathrm{pert}} \\ &+ \frac{1}{a}\sum_{k\in\mathbb{k}} \omega_{\mathrm{MS},k}\boldsymbol{b}^*_k\boldsymbol{b}_k + \frac{1}{6a}\sum_{K\in\mathbb{K}} \omega_{\mathrm{T},K}\boldsymbol{d}^*_K\boldsymbol{d}_K,\end{aligned} \tag{39}$$

where we omitted the trivial unity factors. In the following, we denote the function in the large brackets by $E_{\mathrm{hom}}(a, p_a, \phi, p_\phi)$. $\mathbf{1}_{\mathrm{pert}}$ is the unity operator on $\mathcal{H}_{\mathrm{pert}}$, and this is simply the tensor product of all individual Fock space unities. We emphasize that not only the zeroth order offset energy contribution E_{hom} depends on the homogeneous phase space variables but also the frequency functions $\omega_{\mathrm{MS},k}$ and $\omega_{\mathrm{T},K}$ as well as any of the annihilation and creation operators of the Mukhanov-Sasaki and tensor systems. In the following, we first verify that our model fits into the space adiabatic perturbation scheme and apply the theory subsequently.

III. SPACE ADIABATIC PERTURBATION THEORY

A. Conditions for space adiabatic perturbation theory

To apply SAPT to the cosmological model, the Hamilton constraint symbol $\boldsymbol{C}(a, p_a, \phi, p_\phi)$ in Eq. (39) has to meet certain requirements. We closely follow Panati, Spohn, and Teufel [4,5] although the conditions there are quite restrictive. We will point to occurring difficulties while discussing the following four conditions.

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

$$\mathcal{H} = L^2(\mathbb{R}^n, \mathrm{d}x) \otimes \mathcal{H}_{\mathrm{f}} = L^2(\mathbb{R}^n, \mathcal{H}_{\mathrm{f}}), \tag{40}$$

where $L^2(\mathbb{R}^n, \mathrm{d}x)$ is the state space of the slow subsystem. The state space of the fast subsystem $\mathcal{H}_{\mathrm{f}}$ must be separable.

In the given case, the state space of the homogeneous system which we associate with the "slow" system of SAPT is modeled on $\mathbb{R}^+ \times \mathbb{R}$ since the scale factor can only take values on the positive real line. This will also lead to domain questions when it comes to the definition of certain operators (e.g., the momentum operator $\hat{p}_a$). Nevertheless, we can define the corresponding Hilbert space as $L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}a\mathrm{d}\phi)$, where the measure is the standard Lebesgue measure. We also point to the possibility of using triadlike variables as in Ref. [3] which solves the domain issues mentioned before. The "fast" Hilbert space $\mathcal{H}_{\mathrm{f}}$ will be associated with the perturbative Fock spaces subsumed under $\mathcal{H}_{\mathrm{pert}}$ which is separable. We emphasize that SAPT (implicitly) requires that the Fock spaces for all different representations depending on a and ϕ be the same. As explained earlier this is not granted without further ado. However, the almost canonical transformations that were performed in Sec. II guarantee just that. The next condition is the following.

(C2) *The Hamilton constraint operator* $\hat{\boldsymbol{C}}$ is the Weyl quantization of a function on the slow phase space $\boldsymbol{C}(a, p_a, \phi, p_\phi)$ which belongs to the symbol class $S^m_\rho(\Gamma_{\mathrm{s}}, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ 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 $\boldsymbol{C}(a, p_a, \phi, p_\phi)$ has values in the self-adjoint operators on $\mathcal{H}_{\mathrm{f}}$.

In fact, it is straightforward to perform a Weyl quantization of the symbol $\boldsymbol{C}(a, p_a, \phi, p_\phi)$ in Eq. (39). Therefore, it is most convenient to consider the classical Hamilton constraint C with its components in Eqs. (29)–(31) from which we have obtained the symbol function $\boldsymbol{C}$ by performing standard Fock quantizations. Starting from C, it is useful to consider each of the terms individually and then to perform

a separate Weyl quantization of the homogeneous parts and a Fock quantization of the inhomogeneities. After a tensorial multiplication of the resulting operators and summation, we obtain the final Hamilton operator constraint $\hat{\boldsymbol{C}}$. The same outcome results from Weyl quantizing $\boldsymbol{C}$ in (39).

Then, the question arises whether the symbol $\boldsymbol{C}$ belongs to the correct symbol class alluded to in (C2). The class $S^m_\rho(\Gamma_{\rm hom}, \mathcal{B}(\mathcal{H}_{\rm pert}))$ consists of the functions on $\Gamma_{\rm hom}$ that have values in the bounded operators on $\mathcal{H}_{\rm pert}$, and for which there exists a set of positive constants $C_{\alpha,\beta}$ for every $\alpha, \beta \in \mathbb{N}^2$ such that for every $p := (p_a, p_\phi)$, it holds true that

$$\sup_{q\in\mathbb{R}^+\times\mathbb{R}} \|(\partial_q^\alpha \partial_p^\beta \boldsymbol{C})(q,p)\|_{\mathcal{B}(\mathcal{H}_{\rm pert})} \le C_{\alpha,\beta}(1+p^2)^{\frac{1}{2}(m-\rho|\beta|)}, \tag{41}$$

and $q := (a, \phi)$ is a short form for the configuration variables. It is easy to check that $\boldsymbol{C}$ fails to satisfy these conditions: It is neither a bounded function with respect to a and ϕ nor is it polynomially bounded with respect to p. Besides, it does not have values in the bounded operators on $\mathcal{H}_{\rm pert}$. A possible solution to this problem is to define an adapted auxiliary Hamilton symbol $\boldsymbol{H}_{\rm aux}$ which satisfies these requirements. We have discussed this in great detail in [2] but the idea goes as follows. First, we cut the sums over all possible mode vectors of the Mukhanov-Sasaki and tensor contributions in Eq. (39). This makes the constraint a bounded operator on the associated Fock spaces for some fixed values (q, p). In order to make $\boldsymbol{C}(q, p)$ a bounded function with respect to q and a polynomially bounded function with respect to p, one can replace the scalar and symbol functions appearing in (39) by an accordingly bounded function that agrees, however, with $\mathcal{C}(q, p)$ below a certain threshold value $E_{\rm t}$. This would even make it a bounded function with respect to the momenta p. Although this is not required for satisfying (C2), we will see that condition (C4) requires just that. Hence, we can follow this procedure and obtain a symbol $\boldsymbol{C}_{\rm aux}(q, p)$ that lies in $S^0_0(\Gamma_{\rm hom}, \mathcal{B}(\mathcal{H}_{\rm pert}))$.

While this new auxiliary Hamiltonian satisfies all the conditions alluded to in this section, it is not possible to compare it or its dynamics with the original Hamilton constraint. The latter is an unbounded operator while the former is bounded, and hence the corresponding solutions will not be similar. On the other hand, the SAPT scheme associated with the original Hamiltonian will not obey any convergence results. Nevertheless, we will remain here with the original Hamilton constraint in order to show the principle possibility of applying the SAPT scheme to this model, even if convergence results would need to be implemented by different methods.

Finally, let us stress that in the original SAPT scheme the constraint $\boldsymbol{C}$ is formally split into its power series coefficients with respect to ε. Since both the homogeneous and the inhomogeneous contributions to $\boldsymbol{C}$ depend on ε, either via $E_{\rm hom}$ or via $\omega_{{\rm MS},k}$ and $\omega_{{\rm T},K}$, there are several nonvanishing power series coefficients. Nevertheless, we will subsume the whole constraint $\boldsymbol{C}$ under its zeroth order contribution $\boldsymbol{C}_0$ in order to simplify the task of applying SAPT. This procedure does not change the final result when carefully sorting the contributions *after* the application of SAPT. Since this paper should rather be seen as a first explorative investigation of SAPT for gauge-invariant cosmological perturbation theory, we will defer this task to a later publication and simply set $\boldsymbol{C} \equiv \boldsymbol{C}_0$.

(C3)γ *Gap condition*. For any fixed value $(q, p) \in \mathbb{R}^+ \times \mathbb{R}^3$ of the homogeneous phase space, the spectrum $\sigma(q, p)$ of the Hamilton symbol $\boldsymbol{C}(q, p)$ contains at least one isolated subset $\sigma_{(\nu)}(q, p)$ associated with a fixed set of quantum numbers (ν), which is uniformly bounded from the remainder $\sigma_{\rm rem}(q, p) := \sigma(q, p)\backslash\sigma_{(\nu)}(q, p)$. In particular, the minimal distance between the elements of $\sigma_{(\nu)}$ and the remainder of the spectrum is nonvanishing for every single $(q, p) \in \Gamma_{\rm hom}$. More precisely, there exists an enclosing interval $I(q, p)$ for the relevant part of the spectrum $\sigma_{(\nu)}$ such that for every value (q, p), the distance $\mathrm{dist}[\sigma_{\rm rem}(q, p), I(q, p)]$ is larger than or equal to $C_{\rm g}(1 + p^2)^{\frac{\gamma}{2}}$, where $C_{\rm g} \ge 0$ is the "gap" constant and $\gamma \in \mathbb{R}$.

To discuss $(\mathrm{C3})_\gamma$, let us assume for the time being that $\boldsymbol{C}$ is a physical Hamilton operator, and we are interested in its entire spectrum. From Eq. (39), it is easy to deduce that $\boldsymbol{C}$ admits a discrete spectrum for any fixed $(q, p) \in \Gamma_{\rm hom}$ because the sums over the (generalized) wave vectors in the Hamilton constraint are discrete and so is the spectrum of the number operators $\boldsymbol{b}_k^* \boldsymbol{b}_k$ and $\boldsymbol{d}_K^* \boldsymbol{d}_K$ when applied to vectors in the total Fock space $\mathcal{H}_{\rm pert}$. Any Fock state $\xi_{(n)} \in \mathcal{H}_{\rm pert}$ with finite energy identifies with a finite set of nonvanishing quantum numbers $(n) := \{\ldots, n_{{\rm MS},k_1}, n_{{\rm MS},k_2}, \ldots, n_{{\rm T},\tau,\tilde{k}_1}, n_{{\rm T},\tau,\tilde{k}_2}, \ldots\}$ where we distinguished between the quantum numbers of the Mukhanov-Sasaki and the tensor perturbations, and $k_1, k_2, \tilde{k}_1, \tilde{k}_2, \ldots$ run over $2\pi\mathbb{Z}^3\backslash\{0\}$. We also introduce degeneracy labels which take the possibility of degenerate eigenstates into account, and we denote them by $b = 1, \ldots, d$ for the Mukhanov-Sasaki system and $b' = 1, \ldots, d'$ for the tensor system. To shorten the notation, we integrate the degeneracy labels in $\beta := \{b, b'\}$ and the degeneracy numbers in $\delta := \{d, d'\}$. According to Eq. (39), the discrete eigenvalue problem for any finite set of quantum numbers (n) then has the form

$$\boldsymbol{C}(q,p)\xi_{(n)}(q,p) = E_{(n)}(q,p)\xi_{(n)}(q,p),$$
$$E_{(n)}(q,p) \coloneqq E_{\mathrm{hom}}(q,p) + \frac{1}{a}\sum_{k\in\mathbb{k}} n_{\mathrm{MS},k,b}\omega_{\mathrm{MS},k} + \frac{1}{6a}\sum_{K\in\mathbb{K}} n_{\mathrm{T},K,b'}\omega_{\mathrm{T},K}. \tag{42}$$

The spectrum of $\boldsymbol{C}(q,p)$ thus consists of the set of all energy bands $\{E_{(n)}(q,p)\}_{(n)}$ for all possible combinations of excitation numbers (n). Since these eigenvalue problems are discrete (recall that the wave vectors k and K are discrete), it is always possible to find, at least locally, a region in the homogeneous phase space where the energy band $E_{(\nu)}$ of some fixed set of quantum numbers (ν) is well separated from the remainder. One could hence restrict our problem to such a region but one has then to deal with domain issues with respect to the homogeneous quantization scheme and review it carefully. As a consequence, it is not possible to satisfy the gap condition in a strict sense and we must consequently abandon any convergence results for the time being.

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

According to the discussion of condition (C2), the Hamilton symbol $\boldsymbol{C}(q,p)$ with the correspondent cutoffs is in $S^0_0(\Gamma_{\mathrm{hom}},\mathcal{B}(\mathcal{H}_{\mathrm{pert}}))$. Hence, if we employed the auxiliary Hamiltonian, we would fall into the category $\gamma = 0$, in line with condition $(\mathrm{C3})_\gamma$. As pointed out earlier, we will abandon the convergence of the perturbative series and remain with the original Hamiltonian in the following.

B. Perturbative construction scheme

The space adiabatic perturbation scheme divides into three steps and relies on the existence of the three following symbol functions. For the construction of these symbols, one needs a so-called star or Moyal product $\star$ which is nothing but the operator product of the slow (here homogeneous) quantum theory pulled back to the corresponding phase space. Recall that SAPT relies on a phase space quantization scheme with respect to the homogeneous sector. After providing the construction steps, we define the star product $\star_\varepsilon$ adapted to the given model, which has the form of a formal power series in ε. Given the Hamilton symbol $\boldsymbol{C}(q,p) \in S^0_0$, the SAPT construction steps are given by [4]

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

$$(\mathrm{S1}-1)\ \boldsymbol{\pi}_{(I)}\star_\varepsilon\boldsymbol{\pi}_{(I)} - \boldsymbol{\pi}_{(I)} = \mathcal{O}_0(\varepsilon^{I+1}), \tag{43}$$

$$(\mathrm{S1}-2)\ \boldsymbol{\pi}^*_{(I)} - \boldsymbol{\pi}_{(I)} = \mathcal{O}_0(\varepsilon^{I+1}), \tag{44}$$

$$(\mathrm{S1}-3)\ \boldsymbol{C}\star_\varepsilon\boldsymbol{\pi}_{(I)} - \boldsymbol{\pi}_{(I)}\star_\varepsilon\boldsymbol{C} = \mathcal{O}_0(\varepsilon^{I+1}). \tag{45}$$

It can be shown that the Weyl quantization of a formal resummation of $\boldsymbol{\pi}$ (see [1] 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., $[\hat{\boldsymbol{C}},\hat{\boldsymbol{\Pi}}] = \mathcal{O}_0(\varepsilon^\infty)$. The estimate means that for all $m \in \mathbb{N}$, there exists a constant $C_m \geq 0$ such that $\|[\hat{\boldsymbol{C}},\hat{\boldsymbol{\Pi}}]\|_{\mathcal{B}(\mathcal{H})} \leq C_m\varepsilon^m$.

(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 $\boldsymbol{u} = \sum_{i\geq 0}\varepsilon^i\boldsymbol{u}_i$ such that its restriction to the Ith order $\boldsymbol{u}_{(I)}$ satisfies

$$(\mathrm{S2}-1)\ \boldsymbol{u}^*_{(I)}\star_\varepsilon\boldsymbol{u}_{(I)} - \mathbf{1}_{\mathrm{pert}} = \mathcal{O}_0(\varepsilon^{I+1}), \tag{46}$$

$$(\mathrm{S2}-2)\ \boldsymbol{u}_{(I)}\star_\varepsilon\boldsymbol{u}^*_{(I)} - \mathbf{1}_{\mathrm{pert}} = \mathcal{O}_0(\varepsilon^{I+1}), \tag{47}$$

$$(\mathrm{S2}-3)\ \boldsymbol{u}_{(I)}\star_\varepsilon\boldsymbol{\pi}_{(I)}\star_\varepsilon\boldsymbol{u}^*_{(I)} - \boldsymbol{\pi}_{\mathrm{p}} = \mathcal{O}_0(\varepsilon^{I+1}). \tag{48}$$

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 $\boldsymbol{C}_{\mathrm{eff}} = \sum_{i\geq 0}\varepsilon^i\boldsymbol{C}_{\mathrm{eff},i}$, or more precisely its restriction to the Ith order according to

$$\boldsymbol{C}_{\mathrm{eff},(I)} = \boldsymbol{u}_{(I)}\star_\varepsilon\boldsymbol{C}\star_\varepsilon\boldsymbol{u}^*_{(I)}. \tag{49}$$

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

$$e^{-i\hat{\boldsymbol{C}}t} - \hat{\boldsymbol{u}}^\dagger_{(I)}e^{-i\hat{\boldsymbol{C}}_{\mathrm{eff},(I)}t}\hat{\boldsymbol{u}}_{(I)} = \mathcal{O}_0(\varepsilon^{I+1}|t|). \tag{50}$$

Hence, after unitarily transforming back to the original Hilbert space, the dynamics generated by

$\hat{\boldsymbol{C}}_{\mathrm{eff}}$ corresponds "almost" to the dynamics of the original Hamiltonian $\hat{\boldsymbol{C}}$.

In Appendix, we will be much more precise about the explicit construction steps and give concrete formulas for the relevant computational steps in order to obtain the effective Hamilton symbol up to second order in the adiabatic perturbations. We also refer to [1] for an iterative construction scheme for any desired perturbative order and to [2] for concrete applications of the scheme to simpler models. In the following, we apply SAPT to the cosmological model with gauge-invariant perturbations. We will construct $\boldsymbol{\pi}_{(1)}$ as well as $\boldsymbol{u}_{(1)}$ in order to finally determine $\boldsymbol{C}_{\mathrm{eff},(2)}$.

Therefore, we recall that the perturbation parameter of the scheme is here provided by the dimensionless ratio of the coupling constants, namely by $\varepsilon^2 = \kappa/\lambda$. Since the construction of the space adiabatic symbols is subject to two different perturbative scalings, namely with respect to ε for the homogeneous scalar field and with respect to ε^2 for the homogeneous gravitational degrees of freedom (recall the definition of p_ϕ and p_a), the Moyal product takes for two operator-valued functions $\boldsymbol{A}(q,p), \boldsymbol{B}(q,p) \in S^m_\rho(\Gamma_{\mathrm{hom}}, \mathcal{B}(\mathcal{H}_{\mathrm{pert}}))$ the form

$$(\boldsymbol{A} \star_\varepsilon \boldsymbol{B})(q,p) \approx \Big(\boldsymbol{A} \exp\Big(\frac{i\varepsilon}{2}(\overleftarrow{\partial}_\phi \vec{\partial}_{p_\phi} - \overleftarrow{\partial}_{p_\phi}\vec{\partial}_\phi) - \frac{i\varepsilon^2}{2}(\overleftarrow{\partial}_a \vec{\partial}_{p_a} - \overleftarrow{\partial}_{p_a}\vec{\partial}_a)\Big)\boldsymbol{B}\Big)(q,p), \tag{51}$$

where the vectors indicate the direction in which the partial derivatives act. As we will see in the following, the Moyal product with respect to the gravitational degrees of freedom does not contribute to the computations up to second order in the perturbation scheme. Up to the two different scalings, the scheme proceeds in the lines of [3]. Up to first order, the Moyal product is given by

$$(\boldsymbol{A} \star_\varepsilon \boldsymbol{B})(q,p) = (\boldsymbol{A}\cdot\boldsymbol{B})(q,p) + \frac{i\varepsilon}{2}\{\boldsymbol{A},\boldsymbol{B}\}_{\mathrm{hom}}(q,p) + \mathcal{O}(\varepsilon^3), \tag{52}$$

where we used the Poisson bracket notation $\{\boldsymbol{A},\boldsymbol{B}\}_{\mathrm{hom}} := (\partial_\phi \boldsymbol{A})\cdot(\partial_{p_\phi}\boldsymbol{B}) - (\partial_{p_\phi}\boldsymbol{A})\cdot(\partial_\phi \boldsymbol{B})$. Since we will give all the details regarding the construction scheme in Appendix, we will only provide the most relevant formulas in the following.

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

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

$$\boldsymbol{\pi}_0(q,p) = \sum_{\beta=1}^{\delta_{(\nu)}} \xi_{(\nu)_\beta}(q,p)\langle \xi_{(\nu)_\beta}(q,p), \cdot\rangle_{\mathcal{F}_s}, \tag{53}$$

where $(\nu)_\beta = \{\nu_{k,K,\beta}\}_{k\in\Bbbk, K\in\mathbb{K}}$ is the set of excitation numbers of the chosen Fock state and $\beta = 1,\ldots,\delta_{(\nu)}$ is the associated degeneracy label. The projector symbol $\boldsymbol{\pi}_0(q,p)$ exists for every point $(q,p) \in \Gamma_{\mathrm{hom}}$ for which the energy gap between $E_{(\nu)}(q,p)$ and the remainder of the spectrum persists. Because of the continuity of the map $(q,p) \mapsto \boldsymbol{C}(q,p)$, also $(q,p) \mapsto \boldsymbol{\pi}_0(q,p)$ is continuous. By construction, $\boldsymbol{\pi}_0$ satisfies the construction rules (S1) restricted to the zeroth order in ε. In particular, it satisfies (S1–1) $\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_0 - \boldsymbol{\pi}_0 = 0$, (S1–2) $\boldsymbol{\pi}_0^* = \boldsymbol{\pi}_0$, and (S1–3) $[\boldsymbol{C},\boldsymbol{\pi}_0]_{\mathrm{pert}} = 0$. Consequently, the symbol (53) 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 from above, the rule (S1–1) restricted to its first order components provides an equation for determining the diagonal parts of $\boldsymbol{\pi}_1$, namely

$$\frac{i}{2}\{\boldsymbol{\pi}_0,\boldsymbol{\pi}_0\}_{\mathrm{hom}} + \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1 + \boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0 = \boldsymbol{\pi}_1. \tag{54}$$

This implies that the diagonal contributions can be split into two parts which we define as $\boldsymbol{\pi}_1^{\mathrm{D},0} := \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}^{\mathrm{D},\perp} = \boldsymbol{\pi}_0^\perp\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0^\perp$, where we introduced the orthogonal complement of $\boldsymbol{\pi}_0$, namely $\boldsymbol{\pi}_0^\perp := \mathbf{1}_{\mathrm{pert}} - \boldsymbol{\pi}_0$. As discussed in the companion paper [1], the diagonal part will, however, not enter the computations for the effective Hamilton symbol, and so we omit its further discussion and come to the construction rule (S1–3). This gives the off-diagonal part of $\boldsymbol{\pi}_1$. Its restriction to the first order in ε is given by

$$\frac{1}{2}\{\boldsymbol{C},\boldsymbol{\pi}_0\}_{\mathrm{hom}} - \frac{1}{2}\{\boldsymbol{\pi}_0,\boldsymbol{C}\}_{\mathrm{hom}} + \boldsymbol{C}\cdot\boldsymbol{\pi}_1 - \boldsymbol{\pi}_1\cdot\boldsymbol{C} = 0. \tag{55}$$

We extract the off-diagonal contributions $\boldsymbol{\pi}_1^{\mathrm{OD},1} := \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0^\perp$ and $\boldsymbol{\pi}_1^{\mathrm{OD},2} := \boldsymbol{\pi}_0^\perp\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0$ by multiplying Eq. (55) 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 $\boldsymbol{C}$ by $\boldsymbol{C}^\perp := \boldsymbol{C}\cdot\boldsymbol{\pi}_0^\perp$, and we use that $\boldsymbol{C}\cdot\boldsymbol{\pi}_0 = E_{(\nu)}\mathbf{1}_{\mathrm{pert}}$. This yields for the total symbol $\boldsymbol{\pi}_1 = \boldsymbol{\pi}_1^{\mathrm{OD},1} + \boldsymbol{\pi}_1^{\mathrm{OD},2}$,

$$\boldsymbol{\pi}_1 = -\frac{i}{2}(\boldsymbol{\pi}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{C}+E_{(\nu)}\mathbf{1}_{\mathrm{pert}}\}_{\mathrm{hom}}\cdot(\boldsymbol{C}^\perp - E_{(\nu)}\mathbf{1}_{\mathrm{pert}})^{-1}\cdot\boldsymbol{\pi}_0^\perp + (\boldsymbol{C}^\perp - E_{(\nu)}\mathbf{1}_{\mathrm{pert}})^{-1}\cdot\boldsymbol{\pi}_0^\perp\cdot\{\boldsymbol{\pi}_0,\boldsymbol{C}+E_{(\nu)}\mathbf{1}_{\mathrm{pert}}\}_{\mathrm{hom}}\cdot\boldsymbol{\pi}_0). \tag{56}$$

For a concrete evaluation of $\boldsymbol{\pi}_1$, it is necessary to evaluate the derivatives of the eigenfunctions $\xi_{(n)}(q,p)$ with respect to ϕ and p_ϕ according to the definition of the homogeneous Poisson bracket. Therefore, we use the explicit (q,p)-dependence of the creation operators $\boldsymbol{b}_k^*(q,p)$ and $\boldsymbol{d}_K^*(q,p)$. Therefore, let us start by defining the perturbative states in more detail.

Every excited state in the Hilbert space $\mathcal{H}_{\text{pert}}$ can be constructed from the vacuum state $\Omega(q,p)$ by applying the desired number $(n_{\text{MS},k}, n_{\text{T},k',+}, n_{\text{T},k'',-})$ of creation operators for every set of wave numbers k, k', k''. SAPT chooses formally one such eigenstate with quantum number(s) $(\nu)_\beta$ given by

$$\xi_{(n)}(q,p) = \prod_{k\in\mathbb{k}}\prod_{K\in\mathbb{K}} \frac{(\boldsymbol{b}_k^*)^{n_{\text{MS},k}}}{\sqrt{n_{\text{MS},k}!}} \frac{(\boldsymbol{d}_K^*)^{n_{\text{T},K}}}{\sqrt{n_{\text{T},K}!}} \Omega(q,p), \tag{57}$$

where $\Omega(q,p) \in \mathcal{H}_{\text{pert}}$ is the vacuum state of this representation defined by the requirement to satisfy $\boldsymbol{b}_k(q,p)\Omega(q,p) = 0$ and $\boldsymbol{d}_K(q,p)\Omega(q,p) = 0$ for every $k \in \mathbb{k}$ and $K \in \mathbb{K}$. We introduce the explicit representation of the Mukhanov-Sasaki wave function and the tensor wave functions as a product by

$$\xi_{(n)} =: \xi^{\text{MS}}_{(\nu_{\text{MS}})} \cdot \prod_\tau \xi^{\text{T},\tau}_{(\nu_{\text{T}})}. \tag{58}$$

Recall that the creation and annihilation operators for the Mukhanov-Sasaki and the tensor modes depend explicitly on the homogeneous phase space variables through the masses within the frequency functions,

$$\begin{aligned} \omega_{\text{MS},k}(q,p) &= \varepsilon^2\sqrt{k^2 + M^2_{\text{MS}}(q,p)}, \\ \omega_{\text{T},K}(q,p) &= \varepsilon^2\sqrt{18k^2 + 6(\varepsilon M_{\text{T}})^2(q,p)}. \end{aligned} \tag{59}$$

We deduce the derivatives of the annihilation operators with respect to $\lambda \in \{q,p\}$, namely

$$\begin{aligned} \frac{\partial \boldsymbol{b}_k(q,p)}{\partial\lambda} &:= \alpha^{\text{MS}}_{\lambda,k}(q,p)\boldsymbol{b}_k^*(q,p) \\ &= -\frac{1}{8}\frac{\varepsilon^4\partial_\lambda M^2_{\text{MS}}(q,p)}{\omega^2_{\text{MS},k}(q,p)}\boldsymbol{b}_k^*(q,p), \end{aligned} \tag{60}$$

$$\begin{aligned} \frac{\partial \boldsymbol{d}_K(q,p)}{\partial\lambda} &:= \alpha^{\text{T}}_{\lambda,K}(q,p)\boldsymbol{d}_K^*(q,p) \\ &= -\frac{3}{4}\frac{\varepsilon^6\partial_\lambda M^2_{\text{T}}(q,p)}{\omega^2_{\text{T},k}(q,p)}\boldsymbol{d}_K^*(q,p), \end{aligned} \tag{61}$$

and we implicitly defined the functions $\alpha^{\text{MS}}_{\lambda,k}$ and $\alpha^{\text{T}}_{\lambda,K}$. The defining equations for the vacuum $\Omega(q,p)$, together with the derivatives of the annihilation and creation operators, give rise to a formula for the λ-derivative of the vacuum state

$$\begin{aligned} \frac{\partial\Omega(q,p)}{\partial\lambda} = &\sum_{k\in\mathbb{k}} \alpha^{\text{MS}}_{\lambda,k}(q,p)(\boldsymbol{b}_k^*\boldsymbol{b}_k^*\Omega)(q,p) \\ &+ \sum_{K\in\mathbb{K}} \alpha^{\text{T}}_{\lambda,K}(q,p)(\boldsymbol{d}_K^*\boldsymbol{d}_K^*\Omega)(q,p). \end{aligned} \tag{62}$$

With this, it is straightforward to compute the λ-derivative of any excited state $\xi_{(n)}$ using that $\xi_{(n)}$ can be expressed by application of an appropriate number of creation operators on the vacuum state [see Eq. (57)]. It is convenient (see [1,3]) to express the derivative of the eigenstates with respect to the homogeneous parameters as an application of a connection $\boldsymbol{A}_\lambda \in C^\infty(\Gamma_{\text{hom}}, \mathcal{L}(\mathcal{H}_{\text{pert}}))$ on the global Hilbert bundle H, and we write

$$\begin{aligned} &\frac{\partial\xi_{(n)}(q,p)}{\partial\lambda} =: \boldsymbol{A}_\lambda\xi_{(n)} =: \mathcal{A}^{(m)}_{\lambda(n)}\xi_{(m)}, \\ &\mathcal{A}^{(m)}_{\lambda(n)}(q,p) \in C^\infty(\Gamma_{\text{hom}},\mathbb{R}) \quad \forall\ (n),(m), \end{aligned} \tag{63}$$

where the summation over (m) includes essentially *all* possible excitation numbers within the Fock space $\mathcal{H}_{\text{pert}}$. However, there is only a countable number of (m)'s for which $\mathcal{A}^{(m)}_{\lambda(n)}$ is nonvanishing if (n) is a finite set of nonvanishing excitation numbers. Therefore, let us state again that the notation (n) is a short form for a set of finitely many, nonvanishing excitation numbers that we can write more explicitly as $\{\ldots, n_{\text{MS},k_1}, n_{\text{MS},k_2}, \ldots, n_{\text{T},K_1}, n_{\text{T},K_2}, \ldots\}$. Besides, we denote a set of quantum numbers which only differs from (n) in the single quantum number $n_{\text{MS/T},k/K}$ by ± 2 by $\{\ldots, n_{\text{MS/T},k/K} \pm 2, \ldots\}$. We are therefore led to write the connection coefficients in the direction λ that link the state (n) and the state $\{\ldots, n_{\text{MS/T},k/K} \pm 2, \ldots\}$ as

$$\mathcal{A}_{\lambda n^{\,n_{\text{MS},k,\beta}-2}_{\text{MS},k,\beta}}(q,p) := -\alpha^{\text{MS}}_{\lambda,k}(q,p)\sqrt{(n_{\text{MS},k,\beta}-1)\cdot n_{\text{MS},k,\beta}}, \tag{64}$$

$$\mathcal{A}_{\lambda n^{\,n_{\text{MS},k,\beta}+2}_{\text{MS},k,\beta}}(q,p) := \alpha^{\text{MS}}_{\lambda,k}(q,p)\sqrt{(n_{\text{MS},k,\beta}+1)\cdot(n_{\text{MS},k,\beta}+2)}, \tag{65}$$

$$\mathcal{A}_{\lambda n^{\,n_{\text{T},K,\beta'}-2}_{T,K,\beta'}}(q,p) := -\alpha^{\text{T}}_{\lambda,K}(q,p)\sqrt{(n_{\text{T},K,\beta'}-1)\cdot n_{\text{T},K,\beta'}}, \tag{66}$$

$$\mathcal{A}_{\lambda n^{\,n_{\text{T},K,\beta'}+2}_{\text{T},K,\beta'}}(q,p) := \alpha^{\text{T}}_{\lambda,K}(q,p)\sqrt{(n_{\text{T},K,\beta'}+1)\cdot(n_{\text{T},K,\beta'}+2)}. \tag{67}$$

In this notation, the derivative of some state $\xi_{(n)}(q,p)$ with respect to λ has the form

$$\frac{\partial \xi_{(n)}(q,p)}{\partial \lambda} = \sum_{k\in\mathbb{k}} \Big(\mathcal{A}_{\lambda n_{\mathrm{MS},k,\beta}}^{\;\;n_{\mathrm{MS},k,\beta}-2} \xi^{\mathrm{MS}}_{\{\ldots,n_{\mathrm{MS},k,\beta}-2,\ldots\}} + \mathcal{A}_{\lambda n_{\mathrm{MS},k,\beta}}^{\;\;n_{\mathrm{MS},k,\beta}+2} \xi^{\mathrm{MS}}_{\{\ldots,n_{\mathrm{MS},k,\beta}+2,\ldots\}} \Big) \prod_{\tau} \xi^{\mathrm{T},\tau}_{(n_{\mathrm{T}})} + \xi^{\mathrm{MS}}_{(n_{\mathrm{MS}})} \prod_{\tau} \sum_{k\in\mathbb{k}} \Big(\mathcal{A}_{\lambda n_{\mathrm{T},K,\beta'}}^{\;\;n_{\mathrm{T},K,\beta'}-2} \xi^{\mathrm{T},\tau}_{\{\ldots,n_{\mathrm{T},k,\beta'}-2,\ldots\}} + \mathcal{A}_{\lambda n_{\mathrm{T},K,\beta'}}^{\;\;n_{\mathrm{T},K,\beta'}+2} \xi^{\mathrm{T},\tau}_{\{\ldots,n_{\mathrm{T},k,\beta'}+2,\ldots\}} \Big) \xi^{\mathrm{T},\tau'\neq\tau}_{(n_{\mathrm{T}})}. \tag{68}$$

Coming back to the actual construction scheme, we are now ready to explicitly compute an expression for $\boldsymbol{\pi}_1$ as defined in Eq. (56). The homogeneous Poisson brackets give rise to several derivatives with respect to ϕ and p_ϕ. The derivatives of the symbol functions $\boldsymbol{\pi}_0$, etc., can be obtained by using the Riesz representation used in Eq. (53). Thereby note that the eigenstates, and hence also the connection coefficients, are real valued. A straightforward, but tedious computation (see Appendix), gives

$$\boldsymbol{\pi}_1^{\mathrm{OD}} = \frac{i}{2} \sum_{\beta=1}^{\delta} \sum_{(n)\neq(\nu)_\beta} \frac{A_{(\nu)_\beta(n)}}{E_{(\nu)_\beta} - E_{(n)}} \times \left(\xi_{(\nu)_\beta} \langle \xi_{(n)}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}} - \xi_{(n)} \langle \xi_{(\nu)_\beta}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}} \right), \tag{69}$$

and the function $A_{(\nu)_\beta(n)}(q,p)$ is defined according to

$$A_{(\nu)_\beta(n)} \coloneqq \mathcal{A}^{(n)}_{\phi(\nu)_\beta} \frac{\partial (E_{(n)} + E_{(\nu)_\beta})}{\partial p_\phi} - \mathcal{A}^{(n)}_{p_\phi(\nu)_\beta} \frac{\partial (E_{(n)} + E_{(\nu)_\beta})}{\partial \phi} + (E_{(n)} - E_{(m)}) (\mathcal{A}^{(m)}_{p_\phi(\nu)_\beta} \mathcal{A}^{(n)}_{\phi(m)} - \mathcal{A}^{(m)}_{\phi(\nu)_\beta} \mathcal{A}^{(n)}_{p_\phi(m)}). \tag{70}$$

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 (q,p) 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 $\mathcal{K}_{\mathrm{pert}} \subset \mathcal{H}_{\mathrm{pert}}$.

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

We choose an arbitrary but suitable reference subspace $\mathcal{K}_{\mathrm{pert}} \subset \mathcal{H}_{\mathrm{pert}}$ to which we map the relevant dynamics of the problem. The idea is to select one fixed point $(q_0,p_0) \in \Gamma_{\mathrm{hom}}$. We denote the eigenbasis of $\boldsymbol{C}(q_0,p_0)$ at this point by $\{\zeta_{(n)}\} \coloneqq \{\xi_{(n)}(q_0,p_0)\}$, and we define the reference projection by

$$\boldsymbol{\pi}_{\mathrm{p}} \coloneqq \sum_{\beta=1}^{\delta_{(\nu)}} \zeta_{(\nu)_\beta} \langle \zeta_{(\nu)_\beta}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{71}$$

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 $\boldsymbol{u}(q,p)$ 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

$$\boldsymbol{u}_0(q,p) \coloneqq \sum_{(n)} \zeta_{(n)} \langle \xi_{(n)}(q,p), \cdot \rangle_{\mathcal{F}_{\mathrm{s}}}, \tag{72}$$

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 $\boldsymbol{h}_1 = \boldsymbol{h}_1^*$, and $\boldsymbol{k}_1 = -\boldsymbol{k}_1^*$ such that $\boldsymbol{u}_1 =: (\boldsymbol{h}_1 + \boldsymbol{k}_1) \cdot \boldsymbol{u}_0$. The construction rule (S2–1) serves to determine $\boldsymbol{h}_1$ for our choice of $\boldsymbol{\pi}_{\mathrm{p}}$ and $\boldsymbol{u}_0$. In particular, its restriction to first order is given by

$$\frac{i}{2} \{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_{\mathrm{hom}} + 2\boldsymbol{h}_1 = 0. \tag{73}$$

The Hermitian part of $\boldsymbol{u}_1(q,p)$ is accordingly given in terms of the connection coefficients and the fast eigenstates by

$$\boldsymbol{u}_1^{\mathrm{h}}(q,p) = \frac{i}{4} \sum_{(n),(m),(k)} (\mathcal{A}^{(m)}_{\phi(n)} \mathcal{A}^{(k)}_{p_\phi(m)} - \mathcal{A}^{(m)}_{p_\phi(n)} \mathcal{A}^{(k)}_{\phi(m)}) \zeta_{(n)} \langle \xi_{(k)}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{74}$$

To determine the remaining anti-Hermitian piece, let us consider the construction rule (S2–3). By separating the contribution from the anti-Hermitian part from this rule restricted to first order, we define a new operator $\boldsymbol{K}_1$ such that

$$\boldsymbol{u}_{(1)} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{u}^*_{(1)} - \boldsymbol{\pi}_{\mathrm{p}} =: \varepsilon (\boldsymbol{K}_1 + [\boldsymbol{k}_1, \boldsymbol{\pi}_{\mathrm{p}}]_{\mathrm{pert}}) + \mathcal{O}_0(\varepsilon^2). \tag{75}$$

By expanding the star products in this equation, we obtain an explicit expression for $\boldsymbol{K}_1$ given by

$$\boldsymbol{K}_1 = \boldsymbol{h}_1 \cdot \boldsymbol{\pi}_{\mathrm{p}} + \boldsymbol{\pi}_{\mathrm{p}} \cdot \boldsymbol{h}_1 + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1 \cdot \boldsymbol{u}_0^* + \frac{i}{2} \boldsymbol{u}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{u}_0^*\}_{\mathrm{hom}} + \frac{i}{2} \{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_{\mathrm{hom}} \cdot \boldsymbol{\pi}_{\mathrm{p}}. \tag{76}$$

Using that a solution to $\boldsymbol{k}_1$ arises as $\boldsymbol{k}_1 = -[\boldsymbol{\pi}_\mathrm{p}, [\boldsymbol{K}_1, \boldsymbol{\pi}_\mathrm{p}]_\mathrm{pert}]_\mathrm{pert}$, we finally get

$$\boldsymbol{u}_1 = [\boldsymbol{\pi}_\mathrm{p}, \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1^\mathrm{OD} \cdot \boldsymbol{u}_0^*]_\mathrm{pert} \cdot \boldsymbol{u}_0 + \frac{i}{4}[\boldsymbol{\pi}_\mathrm{p}, \{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_\mathrm{hom}]_\mathrm{pert} \cdot \boldsymbol{u}_0. \tag{77}$$

With the already known solution of $\boldsymbol{\pi}_1$, the solution $\boldsymbol{u}_1$ can be obtained from a simple algebraic computation. More precisely, we have

$$\boldsymbol{u}_1 = \frac{i}{2}\sum_{\beta=1}^{\delta_{(\nu)}} \sum_{(n)\neq(\nu)_\beta} \frac{A_{(\nu)_\beta(n)}}{E_{(\nu)_\beta} - E_{(n)}} \times (\zeta_{(\nu)_\beta}\langle \xi_{(n)}, \cdot\rangle_{\mathcal{F}_\mathrm{s}} + \zeta_{(n)}\langle \xi_{(\nu)_\beta}, \cdot\rangle_{\mathcal{F}_\mathrm{s}}). \tag{78}$$

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

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 Hamiltonian $\hat{\boldsymbol{C}}_\mathrm{eff}$ acting on this subspace is the Weyl quantization of the symbol function $\boldsymbol{C}_\mathrm{eff}$ which obeys the construction rule (S3), namely $\boldsymbol{C}_\mathrm{eff} = \boldsymbol{u}\star_\varepsilon \boldsymbol{C}\star_\varepsilon \boldsymbol{u}^*$. Again, we assume a power series ansatz with respect to ε for the symbol $\boldsymbol{C}_\mathrm{eff}$ that we are going to determine up to second order, i.e., $\boldsymbol{C}_{\mathrm{eff},(1)} = \boldsymbol{C}_{\mathrm{eff},0} + \varepsilon\boldsymbol{C}_{\mathrm{eff},1} + \varepsilon^2\boldsymbol{C}_{\mathrm{eff},2}$. In the following, we restrict our attention to the dynamics within the relevant subspace and thus project $\boldsymbol{C}_{\mathrm{eff},(2)}$ on $\boldsymbol{\pi}_\mathrm{p}$. At zeroth order, this yields

$$\boldsymbol{C}_{\mathrm{eff},0,\mathrm{p}} = \sum_{b,b'=1}^{d,d'} \left(E_\mathrm{hom}(a, p_a, \phi, p_\phi) + \frac{1}{a}\sum_{k\in\mathbb{k}} \nu_{\mathrm{MS},k,b}\omega_{\mathrm{MS},k} + \frac{1}{6a}\sum_{K\in\mathbb{K}} \nu_{\mathrm{T},K,b'}\omega_{\mathrm{T},K}\right)\zeta_{(\nu)_\beta}\langle \zeta_{(\nu)_\beta}, \cdot\rangle_{\mathcal{F}_\mathrm{s}}, \tag{79}$$

which includes the standard zeroth order Hamilton constraint for an FLRW universe with a homogeneous and isotropic scalar field denoted here by $E_\mathrm{hom}(a, p_a, \phi, p_\phi)$, and the bare energy contributions from the relevant energy band $\xi_{(\nu)_\beta}$. Note that these additional terms are finite as we chose the relevant quantum numbers $\{\nu_{\mathrm{MS},k,b}, \nu_{\mathrm{T},K,b'}\}$ to be nonvanishing for only a finite number of wave vectors k and K. If we considered the vacuum state for which any of the numbers $\{\nu_{\mathrm{MS},k,b}, \nu_{\mathrm{T},K,b'}\}$ vanish, there would be no additional contributions to E_hom.

We also note that in the above result E_hom, $\omega_{\mathrm{MS},k}$, $\omega_{\mathrm{T},K}$ as well as $\zeta_{(\nu)_\beta}$ depend on ε by definition. These ε-dependent terms should actually be removed and added to higher order contributions of the effective constraint. Regarding E_hom this task is relatively simple but for the other occurrences of ε the analysis is more difficult because ε appears in summands under a square root. Since, however, the explicit analysis and the finding of quantum solutions for this constraint are not in the scope of this paper, we defer this task to a later publication and continue with the SAPT scheme regardless.

For the first and second order contributions of $\boldsymbol{C}_\mathrm{eff}$, 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. [2,5])

$$\boldsymbol{C}_{\mathrm{eff},1} = \left(\boldsymbol{u}_1 \cdot \boldsymbol{C} - \boldsymbol{C}_{\mathrm{eff},0} \cdot \boldsymbol{u}_1 + \frac{i}{2}\{\boldsymbol{u}_0, \boldsymbol{C}\}_\mathrm{hom} - \frac{i}{2}\{\boldsymbol{C}_{\mathrm{eff},0}, \boldsymbol{u}_0\}_\mathrm{hom}\right) \cdot \boldsymbol{u}_0^*. \tag{80}$$

To evaluate $\boldsymbol{C}_{\mathrm{eff},1}$, recall that $\boldsymbol{u}_1$ has no diagonal contributions. Therefore, $\boldsymbol{C}_{\mathrm{eff},1}$ has no diagonal contributions at all such that $\boldsymbol{C}_{\mathrm{eff},1,\mathrm{p}} \coloneqq \boldsymbol{\pi}_\mathrm{p} \cdot \boldsymbol{C}_{\mathrm{eff},1} \cdot \boldsymbol{\pi}_\mathrm{p}$ vanishes identically. The same strategy for determining $\boldsymbol{C}_{\mathrm{eff},1,\mathrm{p}}$ applies for deriving $\boldsymbol{C}_{\mathrm{eff},2,\mathrm{p}}$.

In fact, the second order effective Hamilton symbol includes several contributions but we will show that only one of them is of second order in the perturbative parameter, and hence relevant. First, notice that at second perturbative order one should also include contributions from the ε^2-scheme of the geometric degrees of freedom (a, p_a). This corresponds to a *first* order contribution in the perturbation scheme with respect to the homogeneous gravitational degrees of freedom. Consequently, $\boldsymbol{C}_{\mathrm{eff},2,\mathrm{p}}$ includes the first order effective Hamilton constraint regarding the gravitational ε^2-scheme. However, we already know that the first order effective Hamilton constraint within the relevant energy band vanishes identically, and so we can simply drop this term. The remaining contributions are due to the ε-scheme with respect to the homogeneous scalar matter field. The first of them arises by computing contributions of the first order Moyal product, and the second from second order contributions to the Moyal product, namely

$$\boldsymbol{C}_{\mathrm{eff},2,\mathrm{p}} = \frac{i}{2}\{\boldsymbol{\pi}_\mathrm{p} \cdot \boldsymbol{u}_1, \boldsymbol{C} + E_{(\nu)}\mathbf{1}_\mathrm{f}\}_\mathrm{hom} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_\mathrm{p} + \boldsymbol{\pi}_\mathrm{p} \cdot ([\boldsymbol{u}_0\star_\varepsilon \boldsymbol{C}]_2 - [E_{(\nu)}\star_\varepsilon \boldsymbol{u}_0]_2) \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_\mathrm{p}, \tag{81}$$

where the square brackets with subscript 2 indicate that the inside is restricted to exactly second order in the perturbative scheme. As it turns out, not all contributions to this operator (which is given in terms of the connection coefficients in Appendix) give terms of second order in ε, and we therefore review their components and select the contributions that effectively enter at second order in the perturbative scheme. The appearance of terms that actually

enter at higher orders in ε stems from the fact that the perturbative Mukhanov-Sasaki and tensor contributions to $\boldsymbol{C}$ are by definition of second order in ε. Nevertheless, it was necessary to include them as zeroth order contributions to make the space adiabatic scheme work at the technical level. This does not undermine the results but a careful analysis of all terms is required. We recall that the effective, (a, p_a, ϕ, p_ϕ)-dependent masses of the Mukhanov-Sasaki and the tensor systems depend polynomially on ε with different exponents, and so will their derivatives with respect to the homogeneous variables. Most importantly, we find by inspecting their explicit expressions in Eqs. (32) and (33) that

$$\frac{\partial(\varepsilon M_{\mathrm{T}})^2}{\partial\phi} \propto \varepsilon^2 a^2 \phi \sim \varepsilon^2, \qquad \frac{\partial M^2_{\mathrm{MS}}}{\partial\phi} \propto \varepsilon \frac{a p_\phi}{p_a} \sim \varepsilon, \tag{82}$$

$$\frac{\partial(\varepsilon M_{\mathrm{T}})^2}{\partial p_\phi} = 0, \qquad \frac{\partial M^2_{\mathrm{MS}}}{\partial\phi} \propto \varepsilon \frac{a p_\phi}{p_a} \sim \varepsilon, \frac{p_\phi^3}{a^6 p_a^2} \sim 1. \tag{83}$$

Since the coefficients of the connection depend directly on these derivatives of the masses, it is straightforward to deduce their dependence on ε, namely

$$\mathcal{A}_{\phi^{(m)}_{(n)}}\Big|_{\mathrm{T}} \propto \frac{\partial_\phi(\varepsilon M_{\mathrm{T}})^2}{18k^2 + 6(\varepsilon M_{\mathrm{T}})^2} \sim \varepsilon^2, \qquad \mathcal{A}_{p_\phi{}^{(m)}_{(n)}}\Big|_{\mathrm{T}} = 0, \tag{84}$$

$$\mathcal{A}_{\phi^{(m)}_{(n)}}\Big|_{\mathrm{MS}} \propto \frac{\partial_\phi M^2_{\mathrm{MS}}}{k^2 + M^2_{\mathrm{MS}}} \sim \varepsilon,$$
$$\mathcal{A}_{p_\phi{}^{(m)}_{(n)}}\Big|_{\mathrm{MS}} \propto \frac{\partial_{p_\phi} M^2_{\mathrm{MS}}}{k^2 + M^2_{\mathrm{MS}}} \sim 1, \tag{85}$$

where the vertical lines with subscripts "MS" and "T" indicate the restriction of the connection coefficients to those which contain only nontrivial factors with respect to the Mukhanov-Sasaki or the tensor perturbations, respectively. In addition, there are several other factors that enter the formula for the effective, second order Hamilton constraint, in particular,

$$E_{(m)} - E_{(n)} \sim \varepsilon^2, \qquad (E_{(m)} - E_{(n)})^{-1} \sim \varepsilon^{-2}, \tag{86}$$

$$\partial_\phi E_{\mathrm{hom}} \propto \varepsilon^2 a^3 \phi \sim \varepsilon^2, \qquad \partial_{p_\phi} E_{\mathrm{hom}} \propto \frac{p_\phi}{a^3} \sim 1. \tag{87}$$

With this information, we examine all terms contributing to $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}$ carefully and identify only one single term which is of order ε^0, and consequently enters at the correct order for our scheme. All other terms include additional factors in ε. This relevant contribution comes from the first order Moyal product expressions and is given by

$$\boldsymbol{C}_{\mathrm{eff},2,\mathrm{p}} = -\sum_{\beta,(n)} \frac{1}{E_{(\nu)_\beta} - E_{(n)}} \mathcal{A}_{\phi^{(n)}_{(\nu)_\beta}}\Big|_{\mathrm{MS}} \mathcal{A}_{\phi^{(\nu)_\beta}_{(n)}}\Big|_{\mathrm{MS}} \left(\frac{\partial E_{\mathrm{hom}}}{\partial p_\phi}\right)^2 \zeta_{(\nu)_\beta} \langle \zeta_{(\nu)_\beta}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{88}$$

The sum over all possible excitation numbers (n) reduces to a sum over the wave modes by evaluating the connection coefficients. In particular, we have that

$$\begin{aligned}
\sum_{(n)} \frac{\mathcal{A}_{\phi^{(n)}_{(\nu)_\beta}}\Big|_{\mathrm{MS}} \mathcal{A}_{\phi^{(\nu)_\beta}_{(n)}}\Big|_{\mathrm{MS}}}{E_{(\nu)_\beta} - E_{(n)}} &= \sum_{k\in\mathbb{k}} \left(-\frac{a}{2\omega_{\mathrm{MS},b}(k^2)} (\mathcal{A}_{\phi\nu_{\mathrm{MS},k,b}}{}^{\nu_{\mathrm{MS},k,b}-2})^2 + \frac{a}{2\omega_{\mathrm{MS},b}(k^2)} (\mathcal{A}_{\phi\nu_{\mathrm{MS},k,b}}{}^{\nu_{\mathrm{MS},k,b}+2})^2 \right) \\
&= \sum_{k\in\mathbb{k}} \frac{a(\alpha^{\mathrm{MS}}_{\phi,k})^2}{2\omega_{\mathrm{MS},b}(k^2)} (-(\nu_{\mathrm{MS},k,b} - 1)\nu_{\mathrm{MS},k,b} + (\nu_{\mathrm{MS},k,b} + 1)(\nu_{\mathrm{MS},k,b} + 2)) \\
&= \sum_{k\in\mathbb{k}} \frac{1}{(k^2 + M_{\mathrm{MS}})^{5/2}} \left(\nu_{\mathrm{MS},k,b} - \frac{1}{2}\right) \frac{9}{2} \frac{m^4 a^3 p_\phi^2}{p_a^2}.
\end{aligned} \tag{89}$$

This result, together with $(\partial_{p_\phi} E_{\mathrm{hom}})^2 = p_\phi^2/a^6$, yields the second order effective Hamilton constraint

$$\boldsymbol{C}_{\mathrm{eff},2,\mathrm{p}}(a, p_a, \phi, p_\phi) = -\sum_{b=1}^{d} \sum_{k\in\mathbb{k}} \frac{1}{(k^2 + M^2_{\mathrm{MS}})^{5/2}} \left(\nu_{\mathrm{MS},k,b} + \frac{1}{2}\right) \frac{9}{2} \frac{m^4 p_\phi^4}{a^3 p_a^2} \zeta_{(\nu)_b} \langle \zeta_{(\nu)_b}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{90}$$

Hence, we recover an explicit expression for the effective Hamilton symbol $\boldsymbol{C}_{\mathrm{eff},(2),\mathrm{p}} = \boldsymbol{C}_{\mathrm{eff},0,\mathrm{p}} + \varepsilon^2 \boldsymbol{C}_{\mathrm{eff},2,\mathrm{p}}$ which includes the backreaction of the perturbative energy band with quantum number $(\nu)_\beta$ on the homogeneous degrees of freedom. Interestingly, the backreaction solely comes from the Mukhanov-Sasaki scalar degrees of freedom. Note that M^2_{MS} as well as $\zeta_{(\nu)_b}$ in Eq. (90) depend on ε, and so there will be certain contributions to $\boldsymbol{C}_{\mathrm{eff},2,\mathrm{p}}$ that are actually of

higher than second order in ε. A careful analysis would be necessary to remove these terms. Here, however, we defer from entering this analysis and postpone it to a later publication.

The final step of the scheme consists in Weyl quantizing this symbol function with respect to the homogeneous sector and in finding an appropriate domain and possible solutions that are annihilated by the constraint. Then, by application of the Weyl quantization of $\boldsymbol{u}_{(2)}$, one can rotate the solutions back to the original Hilbert space, which will be solutions to the original constraint $\hat{\boldsymbol{C}}$ up to errors of order ε^3. The computation of $\boldsymbol{u}_{(2)}$ will be part of a future publication.

Finding solutions to this Hamilton constraint appears to be a difficult task. The symbol contains nontrivial (and nonpolynomial) dependencies on the homogeneous phase space variables, and besides the mass term M^2_{MS} is an *indefinite* function on Γ_{hom} and hence leads to tachyonic instabilities for the solutions of the effective Hamilton symbol. In this respect, let us emphasize that this peculiarity is *not* due to the application of the SAPT scheme itself, but already occurs when introducing standard gauge-invariant perturbation fields in cosmology [21]. Therefore, M^2_{MS} can become negative and hence cancel or even surpass the wave vector squared in the denominator here. Regarding the first case, in particular if a nonpositive mass squared cancels the wave number contribution, we observe that for every wave vector $k \in \mathbb{k}$, there is a (possibly nonconnected) three-dimensional region $\gamma_k \subset \Gamma_{\mathrm{hom}}$ in the four-dimensional homogeneous phase space for which this single summand diverges. Since the summation over k is discrete, we expect the divergent surfaces to lie discretely in Γ_{s}. For the first part of the effective Hamiltonian, we have a finite number of such surfaces while for the second part, we have a countably infinite number of divergent surfaces. In addition, the global (third) factor in $\boldsymbol{C}_{\mathrm{eff,2,p}}$ diverges in the limits $a \to 0$, $p_a \to 0$, and $p_\phi \to \pm\infty$.

Despite these divergencies, we emphasize that the symbol Hamilton constraint still needs to be Weyl quantized. It might still be possible to find appropriate solutions. Of course, the divergencies narrow the set of admissible quantum states for which $\hat{\boldsymbol{C}}_{\mathrm{eff,2,p}}$ is a well-defined quantum operator. Besides, the absolute value of a negative mass term might be larger than the wave vector squared such that the total Hamilton constraint symbol would have imaginary contributions. Hence, the question arises whether the final effective Hamilton operator of the theory is self-adjoint or allows for self-adjoint extensions. It is therefore reasonable to seek strategies to circumvent these problems, and we have discussed such solutions in [1] in great detail. In the next section, we employ one of these solutions by performing a symplectic embedding of the homogeneous phase space.

Let us shortly mention that the sum over the infinite number of modes in the effective Hamiltonian is in fact convergent (in case that we have $M^2_{\mathrm{MS}} > 0$). Also note that the second order effective Hamiltonian contains a Casimir effect–like term: Namely, even if we compute the backreaction of the vacuum, i.e., considering $(\nu) = 0$, there will be backreaction.

IV. POSITIVE MASS RESTRICTED MODEL

In this section, we apply one of the strategies proposed in [1] in order to circumvent the problems associated with the indefinite mass squared functions. In particular, we are going to restrict the classical phase space of the homogeneous degrees of freedom to a set of points $(q, p) \in \Gamma_{\mathrm{hom}}$ for which both the effective Mukhanov-Sasaki effective mass squared $M_{\mathrm{MS}}(q,p)^2$ and the effective tensor mass $M_{\mathrm{T}}(q,p)^2$ are manifestly positive. We achieve this by defining two new sets of homogeneous phase space variables which we denote by (b, q') and (ω, u').

A. Symplectic embedding

For simplicity, we restrict our considerations to the case of a vanishing scalar field potential and zero cosmological constant, i.e., $m = 0 = \Lambda$. Consequently, the model does not represent one of the standard inflationary theories. Then, we consider the rescaled homogeneous variables $(a, p_a\phi, p_\phi)$ with Poisson brackets $\{a, p_a\} = \varepsilon^2$ and $\{\phi, p_\phi\} = \varepsilon$. Referring to the definition of the Mukhanov-Sasaki and tensor mass squared functions in Eqs. (32) and (33), the mass squared functions are given here by

$$M^2_{\mathrm{MS}} = -\frac{1}{18}\frac{p_a^2}{a^2} + \frac{7p_\phi^2}{2a^4} - 18\frac{p_\phi^4}{a^2 p_a^2}, \quad (\varepsilon M_{\mathrm{T}})^2 = \frac{p_a^2}{6a^2}. \tag{91}$$

Note that because of $V = 0$, the variable ϕ is cyclic. Evidently, $(\varepsilon M_{\mathrm{T}})^2(q,p) \geq 0$ is manifestly positive, but this is not the case for $M_{\mathrm{MS}}(q,p)^2$. However, after some algebraic manipulations, we can write M^2_{MS} as a manifestly positive quantity. Therefore, we define $y := ap_a$, and we write

$$M^2_{\mathrm{MS}} = \frac{18}{a^4 y^2}(c_+ y^2 - p_\phi^2)(p_\phi^2 - c_- y^2), \quad \text{with}$$
$$c_\pm^2 = \frac{1}{72}(7 \pm \sqrt{33}) \in \mathbb{R}. \tag{92}$$

Note that the constant parameters $c_\pm$ satisfy the inequalities $c_+ > 1 > c_- > 0$. This tells us that if we require $M^2_{\mathrm{MS}} > 0$, we must constrain p_ϕ^2 by

$$c_+^2 y^2 > p_\phi^2 > c_-^2 y^2. \tag{93}$$

This can most easily be achieved by introducing a new explicit parametrization with the variable w defined by

$$p_\phi =: y\omega, \tag{94}$$

for which we require that $\omega \in I := [-c_+, -c_-] \cup [c_-, c_+]$. With this information, let us introduce the two variables

$$\omega = \frac{p_\phi}{y}, \qquad u' := -y\phi, \tag{95}$$

and pursue the aim to define two canonical sets of which (ω, u') is one. Therefore, we also define $\alpha := \ln a$. By this parametrization, the symplectic structure of the homogeneous subsystem can be pulled back. Dropping total differentials, we obtain

$$\varepsilon^2\Theta = -(a\mathrm{d}p_a + \varepsilon\phi\mathrm{d}p_\phi) = -((\alpha + \varepsilon\phi\omega)\mathrm{d}y - \varepsilon u'\mathrm{d}\omega). \tag{96}$$

It is manifest to identify u' as a new momentum variable and ω as its conjugate variable. Similarly, y can serve as a new momentum variable with conjugate variable $(\alpha + \varepsilon\phi\omega)$. In a final step, it is useful to introduce another canonical transformation. Therefore, we define as a canonical variable

$$b := \exp(\alpha + \varepsilon\phi\omega) = a \cdot \exp\left(\varepsilon\frac{\phi p_\phi}{a p_a}\right). \tag{97}$$

It can easily be checked that the variable q' with $y =: bq'$ serves as a conjugate momentum for b, and in terms of the initial variables, it is given by

$$q' = p_a \cdot \exp\left(-\varepsilon\frac{\phi p_\phi}{a p_a}\right). \tag{98}$$

Note also that the following identity holds:

$$\varepsilon\frac{\phi p_\phi}{a p_a} = -\varepsilon\frac{\omega u'}{bq'}. \tag{99}$$

Then, we can identify the total transformation $T : \mathbb{R}^4 \supset U \ni (\tilde{q}, \tilde{p}) \to (q, p) \in W \subset \mathbb{R}^4$, where U, W are subsets of $\mathbb{R}^4$, which maps the new variables canonically on the initial ones, and which is explicitly given by

$$a = b \cdot \exp\left(\varepsilon\frac{\omega u'}{bq'}\right), \quad p_a = q' \cdot \exp\left(-\varepsilon\frac{\omega u'}{bq'}\right), \tag{100}$$

$$\phi = -\frac{u'}{bq'}, \qquad p_\phi = bq'\omega. \tag{101}$$

We emphasize that in the new space adiabatic perturbation scheme, we can treat q' as p_a with rescaling ε^2 and u' as p_ϕ with rescaling ε. In the new variables, the homogeneous part of the Hamilton constraint E_{hom} and the masses, M^2_{MS}, $(\varepsilon M_{\mathrm{T}})^2$, are given by

$$E_{\mathrm{hom}} = \frac{(q')^2}{2b}\exp\left(-\varepsilon\frac{\omega u'}{bq'}\right)\left(\omega^2 - \frac{1}{6}\right), \tag{102}$$

$$M^2_{\mathrm{MS}} = 18\frac{(q')^2}{b^2}\exp\left(-4\varepsilon\frac{\omega u'}{bq'}\right)(c_+ - \omega^2)(\omega^2 - c_-), \tag{103}$$

$$(\varepsilon M_{\mathrm{T}})^2 = \frac{1}{6}\frac{(q')^2}{b^2}\exp\left(-4\varepsilon\frac{\omega u'}{bq'}\right). \tag{104}$$

Now, both mass squared terms are manifestly positive in terms of the two new canonical sets (b, q') and (ω, u'). Note that b is non-negative and $\omega \in I$ is defined on a union of two compact intervals in $\mathbb{R}$. We emphasize that this restriction of the phase space requires us to properly revise the definition of the integral Weyl quantization procedure and the Moyal product. We will discuss this point in the sequel but first formally apply the space adiabatic scheme to the presented model using the standard Weyl formulas available on the whole real line.

B. Space adiabatic construction scheme

We apply SAPT to the inhomogeneous cosmological model with gauge-invariant perturbations and the appropriate transformations as discussed in Sec. II, but employ the new phase space variables (w, u', b, q'). The Hamilton symbol from (39) expressed with these new variables takes the form

$$\begin{aligned}\boldsymbol{C}(\omega, u', b, q') = {} & E_{\mathrm{hom}}(\omega, u', b, q')\mathbf{1}_{\mathrm{pert}} \\ & + \frac{e^{-\varepsilon\frac{\omega u'}{bq'}}}{b}\left(\sum_{k\in\mathbb{k}}\omega_{\mathrm{MS}}(k^2)\boldsymbol{b}_k^*\boldsymbol{b}_k\right. \\ & \left. + \sum_{K\in\mathbb{K}}\frac{\omega_{\mathrm{T}}(k^2)}{6}\boldsymbol{d}_K^*\boldsymbol{d}_K^*\right),\end{aligned} \tag{105}$$

in close analogy to the original model. The frequency functions $\omega_{\mathrm{MS}}(k^2)$ and $\omega_{\mathrm{T}}(k^2)$ have the same form as before but are expressed in terms of the new variables, as well as similarly for the creation and annihilation operators. Therefore, also the application of SAPT proceeds in the very same manner. The functions $\alpha^{\mathrm{MS}}_{\lambda,k}$ and $\alpha^{\mathrm{T}}_{\lambda,K}$ which serve to quantify the derivatives of the annihilation operators $\boldsymbol{b}_k$ and $\boldsymbol{d}_K$ in the direction $\lambda \in \{\omega, u', b, q'\}$ have the same form with respect to the masses and frequencies as before, and so do the coefficients of the connections $\mathcal{A}^{(m)}_{\lambda(n)}$. The explicit expression in terms of the new variables looks of course different from before. We observe again that the connections relate only states which differ by ± 2 excitations in one quantum number.

Since all formal expressions are identical to the ones in Sec. III, we are content to directly present the expression

for the effective Hamilton constraint up to second order in the perturbations. As before, we therefore define an operator-valued symbol $\boldsymbol{\pi}_{\mathrm{p}}$ associated with the fast eigensolution(s) $\zeta_{(\nu)_\gamma} \coloneqq \xi_{(\nu)_\gamma}(w_0, u_0', b_0, q_0') \in \mathcal{H}_{\mathrm{pert}}$ at some fixed phase space point $(w_0, u_0', b_0, q_0') \in \Gamma_{\mathrm{hom}}$. Thereby, we allow for degenerate eigenstates with degeneracy labels $\gamma = (c, c')$ and the degrees of degeneracy $\delta = (d, d')$ for the Mukhanov-Sasaki and the tensor perturbations, respectively. At zeroth order, the scheme generates the standard Born-Oppenheimer result that we directly restrict to the relevant subspace associated with $\boldsymbol{\pi}_{\mathrm{p}}$,

$$\boldsymbol{C}_{\mathrm{eff},0,\mathrm{p}} = \sum_{c,c'=1}^{d,d'} \Bigg(E_{\mathrm{hom}}(\omega, u', b, q') + \frac{e^{-\varepsilon\frac{\omega u'}{bq'}}}{b} \Bigg(\sum_{k\in\mathbb{k}} \nu_{\mathrm{MS},k,c}\,\omega_{\mathrm{MS}}(k^2) + \sum_{K\in\mathbb{K}} \nu_{\mathrm{T},K,c'}\,\frac{\omega_{\mathrm{T}}(k^2)}{6} \Bigg) \Bigg) \cdot \zeta_{(\nu)_\gamma} \langle \zeta_{(\nu)_\gamma}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{106}$$

The first contribution is simply the standard FLRW Hamiltonian constraint. The two remaining contributions correspond to the bare energy of the chosen excitation number (ν) associated with the Mukhanov-Sasaki and the tensor perturbations. At first order of the scheme, the effective Hamilton constraint vanishes. This is because we assumed that the standard Moyal product applies to the given case, and hence the formulas from the previous section and Appendix can be used. In this case, the first order effective Hamiltonian vanishes identically. At second order, it is again possible to split the contributions into a part that only contains the bare symbols and their Poisson brackets, and a part which involves the second order Moyal product. The symbolic form of the first part evidently remains the same, and we only need to replace the Poisson brackets with respect to the old variables by the Poisson brackets with respect to the new variables. We refer to the previous section for the explicit computations. Analogously, it turns out that many contributions are actually of higher order in ε and can thus be omitted for our choice of truncation. This yields

$$\frac{i}{2}\{\boldsymbol{\pi}_{\mathrm{p}}\cdot\boldsymbol{u}_1, \boldsymbol{C} + E_{(\nu)}\mathbf{1}_{\mathrm{pert}}\}_{\mathrm{hom}}\cdot\boldsymbol{u}_0\cdot\boldsymbol{\pi}_{\mathrm{p}} = -b\exp\left(\varepsilon\frac{\omega u'}{bq'}\right)\sum_{c,c'=1}^{d,d'} \zeta_{(\nu)_\gamma}\langle\zeta_{(\nu)_\gamma},\cdot\rangle_{\mathcal{F}_{\mathrm{s}}}\Bigg(\sum_{k\in\mathbb{k}}\frac{2\nu_{\mathrm{MS},k,c}+1}{64\omega_{\mathrm{MS}}(k^2)^5}\cdot\left(\frac{\partial M_{\mathrm{MS}}^2}{\partial u'}\frac{E_{\mathrm{hom}}}{\partial\omega} - \frac{\partial M_{\mathrm{MS}}^2}{\partial\omega}\frac{\partial E_{\mathrm{hom}}}{\partial u'}\right)^2 + \sum_{K\in\mathbb{K}}\frac{27}{8}\frac{2\nu_{\mathrm{T},K,c'}+1}{\omega_{\mathrm{T}}(k^2)^5}\cdot\left(\frac{\partial(\varepsilon M_{\mathrm{T}})^2}{\partial u'}\frac{\partial E_{\mathrm{hom}}}{\partial\omega}\right)^2\Bigg). \tag{107}$$

In contrast to the result using the original variables, the tensor modes generate second order backreaction. This is not very surprising. Even if the two sets of variables are classically related by a canonical embedding, the quantum theories lead to different physical theories. This is a well-known feature of standard quantum theory, and only the comparison with experimental data provides the means to distinguish the physically relevant from the nonrelevant theories.

A priori, the scheme includes also contributions to the second order effective Hamilton constraint that are due to the second order Moyal product. However, as before it turns out that these contributions are all of higher than second order in ε, and hence are not relevant for our computations. This finally yields the effective Hamiltonian with respect to the transformed variables (b, q, ω, u), i.e., without the ε-scaling for the momentum variables. It is important to note that because we use these unscaled variables (b, q, ω, u) the expression for the Hamiltonian can and will in fact depend explicitly on ε. If we used the original variables (b, q', ω, u') (similar to what we have done in all previous examples) with $q' = \varepsilon^2 q$ and $u' = \varepsilon u$, there would be no explicit dependence on ε for the zeroth order part (106) and only a global factor ε^2 for the second order contribution (107). Expressing the latter explicitly as a function of the transformed variables, we obtain

$$\boldsymbol{C}_{\mathrm{eff},(2),\mathrm{p}} = \sum_{c,c'=1}^{d,d'} \zeta_{(\nu)_\gamma}\langle\zeta_{(\nu)_\gamma},\cdot\rangle_{\mathcal{F}_{\mathrm{s}}}\cdot\Bigg(\frac{1}{2}\frac{\varepsilon^2 q^2}{b^2}\exp\left(-\frac{\omega u}{bq}\right)\left(\omega^2 - \frac{1}{6}\right) + \frac{\exp\left(-\frac{\omega u}{bq}\right)}{b}\Bigg(\sum_{k\in\mathbb{k}}\sqrt{k^2 + M_{\mathrm{MS}}^2}\,\nu_{\mathrm{MS},k,c} + \frac{1}{6}\sum_{K\in\mathbb{K}}\sqrt{18k^2 + 6(\varepsilon M_{\mathrm{T}})^2}\,\nu_{\mathrm{T},K,c'}\Bigg) + \sum_{k\in\mathbb{k}}\frac{2\nu_{\mathrm{MS},k,c}+1}{(k^2+M_{\mathrm{MS}}^2)^{5/2}}h_{\mathrm{MS}}(\omega,u,b,q) + \sum_{K\in\mathbb{K}}\frac{2\nu_{\mathrm{T},K,c'}+1}{(18k^2+6(\varepsilon M_{\mathrm{T}})^2)^{5/2}}h_{\mathrm{T}}(\omega,u,b,q)\Bigg), \tag{108}$$

where now the variables u and q refer to the ε-freed u' and q' variables, and we introduced the Hamiltonian backreaction functions

$$h_{\mathrm{MS}} = \exp\left(-13\frac{\omega u}{bq}\right)\left(-\frac{81\varepsilon^{12}q^6\omega^4}{64b^7}\right)(2c_+\omega^2 + c_-(-8c_+ + 2\omega^2 + 1) + c_+ + 4\omega^4 - 2\omega^2)^2,$$
$$h_{\mathrm{T}} = -\exp\left(-13\frac{\omega u}{bq}\right)\cdot\frac{3\varepsilon^{12}q^6\omega^4}{2b^7}. \tag{109}$$

We emphasize again that these expressions are indeed of zeroth and of second order, respectively, in ε with respect to the *ε-scaled* variables (b, q', ω, u') and that the explicit dependence on ε in the previous equations only appears because we used the unscaled variables (b, q, ω, u).

Again, we identify the standard purely homogeneous and isotropic Hamilton constraint of our cosmological model in the first line of this result. Together with the bare energy band contributions from the Mukhanov-Sasaki and tensor perturbations in the ensuing line, this yields the zeroth order contribution of our perturbative scheme. The last line shows the second order contributions of the scheme. These depend partly on the relevant excitation numbers that we have chosen, but there are also contributions which do not, and hence, present a vacuum backreaction from the perturbative degrees of freedom on the homogeneous degrees of freedom. Note that effectively, after having performed a transformation to the unscaled momenta (u, q), they both enter with a factor ε^{12}, and terms containing polynomials of them should thus remain very small within our perturbative scheme.

An interesting question that arises for this model is that of conformal invariance. In fact, we did not consider any conformal coupling to curvature here but it would be interesting to know whether the SAPT corrections preserve such a classical conformal invariance or contribute to the trace anomaly. We leave this for future investigation.

Finally, we emphasize once again that we do not expect the same results as for the previous model without the transformations in the homogeneous sector. Another reason for this to happen is that the restriction to the positive mass region is accomplished by a symplectic embedding rather than a symplectomorphism which in particular changes the entire topology of the slow phase space. Thus, the quantum theories cannot be unitarily equivalent. Note that even if the phase spaces were the same and the transformation was strictly canonical, the quantum theories are likely to differ.

C. Review of the quantization procedure

As shown in Sec. IV A, the symplectic embedding employed there restricts the variable ω to the union of two compact intervals on the real line $I = I_1 \cup I_2 := [-c_+, -c_-] \cup [c_-, c_+]$. The standard Weyl quantization procedure is, however, defined for systems with the cotangent bundle over the real line (or products thereof) as their phase space, and hence, the Weyl quantization procedure is *a priori* not available for this model. In particular, the Moyal product underlying the SAPT scheme might be subject to modifications which would consequently alter the results obtained so far.

There are now two possible strategies. For the first possibility, we take the restriction of the phase space seriously and try to define a Weyl quantization scheme for that model. One would need to redefine the integral representation of the Weyl quantization scheme and possibly define a new form of operator kernels. Since the classical observables as well as the wave functions are only defined on a compact configuration space (or rather a sum of compact spaces), it necessitates the use of a discrete Fourier series with respect to the respective modes instead of the continuous Fourier transform when defining Weyl quantization. It effectively corresponds to considering the phase space $T^*S^1 \oplus T^*S^1$ instead of $T^*\mathbb{R}^2$. It is also important to note that due to the restriction to a finite interval, ambiguities occur in the definition of the momentum operator as it admits an infinite number of self-adjoint extensions [69]. This must also be taken into account when considering the direct sum of two T^*I (we will be more precise in the next paragraph). We also refer to the work by [70] in this respect. In order to recover, the correct product formula for operators and hence a star product on the space of symbol functions, it is advisable to follow the detailed proof for the standard Weyl product formula by Folland [68]. We refrain here from performing this computation and refer to the work by Stottmeister and Thiemann [45] in which such a restricted Weyl quantization in application to LQC has been discussed.

The second possibility is to perform yet another transformation that maps the two intervals on the real line, respectively. Therefore, note that the Hilbert space $L^2(I, \mathrm{d}w)$ of square integrable functions ψ over I is uniquely specified by the restrictions $\psi_1 = \psi_{|I_1}$ and $\psi_2 = \psi_{|I_2}$ which shows that $L^2(I, \mathrm{d}\omega) = L^2(I_1, \mathrm{d}\omega) \oplus L^2(I_2, \mathrm{d}\omega)$. Now each I_k is of the form $[a, b]$ and using suitable maps, one can define new variables. Let us consider for example

$$\omega = f(x) = a + \left(1 + 2\frac{\arctan(x)}{\pi}\right)\frac{b-a}{2}, \tag{110}$$

for which it is true that $\frac{\mathrm{d}f}{\mathrm{d}x}(x) > 0$. The associated conjugate momentum is given by

$$y := u' \frac{\partial f}{\partial x}, \qquad \text{i.e.,} \qquad u' = y \left(\frac{\partial f}{\partial x}\right)^{-1}, \quad (111)$$

and we can easily check that indeed the canonical structure passes over to the new variables, $\{x, y\} = 1$. As a consequence, we may think of $T^* I_k$ as $T^*\mathbb{R}$. We pick the Hilbert space $L^2([a, b], \mathrm{d}\omega)$ on which ω acts by multiplication and u as the derivative operator $-i\frac{\partial}{\partial \omega}$ of course subject to boundary conditions to make it self-adjoint. On the other hand, we can promote the variables x and y to quantum operators such that the latter satisfy the standard commutation relation $[\hat{x}, \hat{y}] = i\hat{1}_{\mathrm{hom}}$. One can thus think of $\hat{x}$ as a multiplication operator and $\hat{y}$ as the $(-i)$-scaled derivative operator with respect to x. Since x and y are defined on the whole $\mathbb{R}^2$, it is reasonable to impose a symmetric Weyl quantization scheme in order to connect with the previous considerations.

Namely, let us consider the symmetric operators $\hat{q} := f^{-1}(\omega)$ and $\hat{p} := \sqrt{f'(x)} u \sqrt{f'(x)}|_{x=f^{-1}(\omega)}$ which satisfy the canonical commutation relations $[\hat{q}, \hat{p}] = -i$ and the unitary map

$$U : L^2([a, b], \mathrm{d}\omega) \to L^2(\mathbb{R}, \mathrm{d}x) : \psi \mapsto \sqrt{f'(x)}\psi(f(x)) = \hat{\psi}(x), \quad (112)$$

with inverse $(U^{-1}\hat{\psi})(\omega) = (\hat{\psi}/\sqrt{f'})(f^{-1}(\omega))$. Then one may check that $\hat{Q} = U\hat{q}U^{-1}$ acts by multiplication by x and $\hat{P} = U\hat{p}U^{-1}$ by $i\partial/\partial x$. Now in every symbol, we express u' and ω in terms of x and y and use their Weyl quantization for $\hat{Q}, \hat{P}$ on $L^2(\mathbb{R}, \mathrm{d}x)$. Using the above formulas, the result may then be translated back in terms of $u', \omega, L^2([a, b], \mathrm{d}\omega)$. For instance, the Weyl quantization of $u'\omega = f(x)/f'(x)y$ on $L^2(\mathbb{R}, \mathrm{d}x)$ yields

$$\begin{aligned}
&\frac{1}{2}[f(\hat{Q})/f'(\hat{Q})\hat{P} + \hat{P}f(\hat{Q})/f'(\hat{Q})] \\
&= \frac{1}{2}U[f(q)/f'(q)p + pf(q)/f'(q)]U^{-1} \\
&= \frac{1}{2}U\left[w/\sqrt{f'(f^{-1}(\omega))}u'\sqrt{f'(f^{-1}(\omega))}\right. \\
&\quad \left. + \sqrt{f'(f^{-1}(\omega))}u'\Big/\sqrt{f'(f^{-1}(\omega))}\omega\right]U^{-1} \\
&= \frac{1}{2}(\omega u' + u'\omega + \omega/\sqrt{f'(f^{-1}(w))}\left[u', \sqrt{f'(f^{-1}(\omega))}\right] \\
&\quad - \left[\omega, \sqrt{f'(f^{-1}(w))}/\sqrt{f'(f^{-1}(\omega))}\omega\right]U^{-1} \\
&= U\frac{1}{2}(u'\omega + \omega u')U^{-1}, \quad (113)
\end{aligned}$$

which shows that Weyl quantization of uw on $L^2([a, b], \mathrm{d}\omega)$ yields the expected symmetric result. Concluding, we simply have to rewrite the formulas of the previous section given there in terms of (a, p_a, ϕ, p_ϕ) now in terms of (b, q', ω, u') and symmetrically order the outcome of the space adiabatic perturbation analysis as if (ω, u') would take values in $\mathbb{R}$. The quantization of (ω, u') takes place on $L^2([-c_+, -c_-], \mathrm{d}\omega) \oplus L^2([c_-, c_+], \mathrm{d}\omega)$.

V. CONCLUSION AND OUTLOOK

In this paper, we applied SAPT to quantum cosmological perturbation theory and demonstrated that the challenges due to the QFT nature of the problem for which SAPT was not designed can be faced squarely. What we now have at our disposal is the machinery to compute the corrections from every energy band of the inhomogeneous Fock space to the effective homogeneous Hamiltonian, in principle to arbitrary adiabatic order. Here, we carried out this program to second adiabatic order. While the computations are rather tedious already to this order, it is clear how to proceed to arbitrary order; the scheme is similar in nature to standard textbook quantum mechanical perturbation theory of pure point spectra.

The treatment of the backreaction problem beyond the semiclassical regime, which we believe to be very important especially in the Planck era of the Universe where we expect the semiclassical approximation to be poor, has revealed many new interesting challenges, including Hilbert-Schmidt conditions that require the mixture of homogeneous and inhomogeneous degrees of freedom in which to formulate the QFT, Weyl-Moyal calculus to feed the quantum nature of the background into the Fock space construction of the inhomogeneous sector, tachyons, and their avoidance and adiabatic backreactions of the Casimir type. Note that, in contrast to the plain Casimir term in quantum electrodynamics, this contribution converges. It is not clear from the current status of the calculations that this also happens at higher adiabatic order in which case presumably also nontrivial renormalization would be required.

What is left to do is to evaluate the phenomenological consequences of this computation and to compare to similar ones in the literature, which mostly focuses on the vacuum energy band. From the explicit expression of our end result, it is evident that the corrections to the effective homogeneous contribution of the Hamiltonian constraint that one unambiguously obtains from the space adiabatic treatment of the backreactions are, unsurprisingly, of a rather new type not previously encountered in more semiclassical treatments [37–39], and it will be interesting to see how these terms affect the previous analysis of the effective dynamics.

In particular, in view of [54] we are in the position to use the standard Schrödinger representation to quantize the effective homogeneous Hamiltonian which in view of the Weyl quantization techniques used by SAPT is more natural than the LQC representation and not plagued by discretization ambiguities as one can directly quantize

position and momentum operators rather than Weyl element approximants. The results of this investigation are reserved for a future publication.

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APPENDIX: SPACE ADIABATIC CONSTRUCTION SCHEME

In this Appendix, we provide the detailed algebraic relations that led to the formulas for the space adiabatic construction scheme. The considerations are general in the sense that they apply to any system that satisfies the conditions (C1)–(C4). We therefore identify the system associated before with the homogeneous sector as the "slow" system (and label it with the letter "s"), and the inhomogeneous system as the "fast" subsystem (labeling it with the letter "f"). We restrict ourselves to second order in the adiabatic perturbations.

1. Construction of the Moyal projector

We recall that the goal of the first step is to construct the symbol function $\boldsymbol{\pi}(q,p)$ associated with a projection operator $\hat{\mathbf{\Pi}}$ that commutes up to small errors in ε with a full Hamilton operator $\hat{\boldsymbol{H}}$ (or constraint). In order to construct the effective Hamilton symbol $\boldsymbol{h}_{\mathrm{eff},(2),\mathrm{p}}$ up to second order in ε, it suffices to construct the first order symbol $\boldsymbol{\pi}_{(1)} \coloneqq \boldsymbol{\pi}_0 + \varepsilon\boldsymbol{\pi}_1$. We recall that conditions (C2) and $(\mathrm{C3})_\gamma$ assure that the zero order Hamilton symbol $\boldsymbol{H}_0(q,p)$ admits a discrete eigenbasis $\{\xi_n(q,p)\}_n$ which serves as a good starting point for the construction of the Moyal projector. n is the short form for any set of excitation numbers here. In particular, the eigenvalue problem has the form

$$\boldsymbol{H}_0(q,p)\xi_n(q,p) = E_n(q,p)\xi_n(q,p), \qquad \xi_n(q,p) \in \mathcal{H}_\mathrm{f}. \tag{A1}$$

Since these eigenvalue problems appear to be "fibered" over the homogeneous phase space, it is convenient to introduce the notion of a gauge connection $\boldsymbol{\mathcal{A}}$ similar to the definition in the theory of fiber bundles for Hilbert bundles. More precisely, we define

$$\begin{aligned}(\nabla\xi)_n(q,p) &\coloneqq (\boldsymbol{\mathcal{A}}\xi)_n(q,p)\\ &= \mathcal{A}_{qn}{}^m(q,p)\xi_m(q,p)\otimes \mathrm{d}q\\ &\quad + \mathcal{A}_{pn}{}^m(q,p)\xi_m(q,p)\otimes \mathrm{d}p.\end{aligned} \tag{A2}$$

To determine the components $\mathcal{A}_{qn}{}^m$ and $\mathcal{A}_{pn}{}^m$ for any n, $m \in \mathbb{N}$, it suffices to compute the partial derivatives of $\xi_n(q,p)$ with respect to q and p, namely we define

$$\frac{\partial\xi_n(q,p)}{\partial\rho} \coloneqq \mathcal{A}_{\rho n}{}^m(q,p)\xi_m(q,p), \qquad \rho \in \{q,p\}. \tag{A3}$$

Let us assume that the eigenfunctions $\xi_n(q,p)$ are real valued for any $n \in \mathbb{N}$, as well as the coefficient functions $\mathcal{A}_{\rho n}{}^m(q,p)$ for any $\rho \in \{q,p\}$ and n, $m \in \mathbb{N}$. By deriving the orthonormality relation $\langle\xi_n,\xi_m\rangle_\mathrm{f} = \delta_{n,m}$ with respect to ρ (which obviously yield zero), where the angular brackets denote the inner product in $\mathcal{H}_\mathrm{f}$, we obtain that the connection is antisymmetric,

$$\mathcal{A}_{\rho n}{}^m = -\mathcal{A}_{\rho m}{}^n. \tag{A4}$$

As a consequence, the connection cannot have any diagonal contributions, namely $\mathcal{A}_{\rho n}{}^n = 0$ for every $n \in \mathbb{N}$. These results and definitions will prove useful for the space adiabatic scheme because the Moyal product of the phase space quantization involves the derivatives of several operator-valued functions with respect to q and p, and we are going to express them in terms of the connection coefficients.

By choosing one physically appropriate eigenstate $\xi_\nu(q,p) \in \mathcal{H}_\mathrm{f}$, the scheme suggests to define the zeroth order projection symbol as

$$\boldsymbol{\pi}_0(q,p) \coloneqq \xi_\nu(q,p)\langle\xi_\nu(q,p),\cdot\rangle_\mathrm{f}. \tag{A5}$$

It is straightforward to check that this symbol satisfies the conditions (S1) at zeroth order by construction, namely

$$\begin{aligned}&(\mathrm{S1}-1)\ \boldsymbol{\pi}\cdot\boldsymbol{\pi}_0 - \boldsymbol{\pi}_0 = 0, \qquad (\mathrm{S1}-2)\ \boldsymbol{\pi}_0^* = \boldsymbol{\pi}_0,\\ &(\mathrm{S1}-3)\ [\boldsymbol{\pi}_0,\boldsymbol{H}_0]_\mathrm{f} = 0,\end{aligned} \tag{A6}$$

and we assume that the wave functions $\xi_n(q,p)$ are real valued. To construct $\boldsymbol{\pi}_1(q,p)$, the scheme divides the symbol into a diagonal part and an off-diagonal part. The following, first condition determines the diagonal part.

a. Condition (S1–1): $\boldsymbol{\pi}\star_\varepsilon\boldsymbol{\pi}-\boldsymbol{\pi}=\mathbf{0}$

By means of the series expansion of $\boldsymbol{\pi}_{(1)}$ and the star product in Eq. (51), the expansion of the first condition (S1–1) in ε yields up to first order

$$\begin{aligned}&\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_0 + \varepsilon\left(\frac{i}{2}\{\boldsymbol{\pi}_0,\boldsymbol{\pi}_0\}_\mathrm{s} + \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1 + \boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0\right)\\ &\quad = \boldsymbol{\pi}_0 + \varepsilon\boldsymbol{\pi}_1 + \mathcal{O}_0(\varepsilon^2).\end{aligned} \tag{A7}$$

Comparing the terms of the same order in ε on both sides, the zeroth order contributions yield the equation $\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_0 = \boldsymbol{\pi}_0$ which is simply (S1–1). The first order contributions determine the diagonal contribution to $\boldsymbol{\pi}_1$ by requiring that

$$0 = \boldsymbol{a}_1 + \boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0 + \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1 - \boldsymbol{\pi}_1, \text{ with } \boldsymbol{a}_1 \coloneqq \frac{i}{2}\{\boldsymbol{\pi}_0,\boldsymbol{\pi}_0\}_\mathrm{s}, \tag{A8}$$

where we tie in with the notation of the general construction scheme in Sec. III. The evaluation of the symbol $\boldsymbol{a}_1$ requires one to build the q- and p-derivatives of $\boldsymbol{\pi}_0(q,p)$. Using the connection components $\mathcal{A}_{\rho n}{}^{m}(q,p)$ from above and the functional representation of $\boldsymbol{\pi}_0$ due to Riesz in Eq. (A5), we obtain

$$\frac{\partial \boldsymbol{\pi}_0}{\partial \rho} = \mathcal{A}_{\rho\nu}{}^{m}(\xi_\nu\langle\xi_m,\cdot\rangle_{\mathrm{f}} + \xi_m\langle\xi_\nu,\cdot\rangle_{\mathrm{f}}), \tag{A9}$$

and we emphasize that ν is a fixed number while we sum over $m \in \mathbb{N}$. We recall that $\langle\cdot,\cdot\rangle_{\mathrm{f}}$ is the inner product within the fast Hilbert space $\mathcal{H}_{\mathrm{f}}$. Using that $\mathcal{A}_{\rho n}{}^{m}$ has no diagonal contributions, this gives for the symbol $\boldsymbol{a}_1$

$$\boldsymbol{a}_1 = \frac{i}{2}\left[\frac{\partial \boldsymbol{\pi}_0}{\partial q}, \frac{\partial \boldsymbol{\pi}_0}{\partial p}\right]_{\mathrm{f}} = \mathcal{A}_{q\nu}{}^{m}\mathcal{A}_{p\nu}{}^{k}(\xi_m\langle\xi_k,\cdot\rangle_{\mathrm{f}} - \xi_k\langle\xi_m,\cdot\rangle_{\mathrm{f}}). \tag{A10}$$

The total diagonal contribution $\boldsymbol{\pi}_1^{\mathrm{D}}$ of $\boldsymbol{\pi}_1$ can be expressed by means of $\boldsymbol{a}_1$ by multiplying with $\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}_0^{\perp} = \mathbf{1}_{\mathrm{f}} - \boldsymbol{\pi}_0$ from the left and the right such that

$$\boldsymbol{\pi}_1^{\mathrm{D}} = -\boldsymbol{\pi}_0\cdot\boldsymbol{a}_1\cdot\boldsymbol{\pi}_0 + \boldsymbol{\pi}_0^{\perp}\cdot\boldsymbol{a}_1\cdot\boldsymbol{\pi}_0^{\perp} = \boldsymbol{\pi}_0^{\perp}\cdot\boldsymbol{a}_1\cdot\boldsymbol{\pi}_0^{\perp}, \tag{A11}$$

where the first term vanishes because, again, the connection has no diagonal terms. In order to determine the remaining off-diagonal part $\boldsymbol{\pi}_1^{\mathrm{OD}} \coloneqq \boldsymbol{\pi}_1 - \boldsymbol{\pi}_1^{\mathrm{D}}$, we consider condition (S1–3).

b. Condition (S1–3): $H\star_\varepsilon\pi - \pi\star_\varepsilon H = 0$

The expansion of (S1–3) up to first order in ε yields the determining equation for $\boldsymbol{\pi}_1^{\mathrm{OD}}$,

$$[\boldsymbol{H}_0,\boldsymbol{\pi}_0]_{\mathrm{f}} + \varepsilon\left(\frac{i}{2}\{\boldsymbol{H}_0,\boldsymbol{\pi}_0\}_{\mathrm{s}} - \frac{i}{2}\{\boldsymbol{\pi}_0,\boldsymbol{H}_0\}_{\mathrm{s}} + \boldsymbol{H}_0\cdot\boldsymbol{\pi}_1 - \boldsymbol{\pi}_1\cdot\boldsymbol{H}_0\right) = \mathcal{O}_0(\varepsilon^2). \tag{A12}$$

Again, the zeroth order contribution is trivially satisfied $[\boldsymbol{H}_0,\boldsymbol{\pi}_0]_{\mathrm{f}} = 0$ as the symbol $\boldsymbol{\pi}_0$ is an orthogonal projection operator on the eigensolutions of $\boldsymbol{H}_0$. Regarding the first order contributions, the scheme requires that the term in the brackets vanishes, in particular,

$$0 \overset{!}{=} -\boldsymbol{b}_1 + [\boldsymbol{H}_0,\boldsymbol{\pi}_1]_{\mathrm{f}}, \quad \text{with}$$
$$\boldsymbol{b}_1 \coloneqq \frac{i}{2}(\{\boldsymbol{H}_0,\boldsymbol{\pi}_0\}_{\mathrm{s}} - \{\boldsymbol{\pi}_0,\boldsymbol{H}_0\}_{\mathrm{s}}). \tag{A13}$$

The off-diagonal contributions $\boldsymbol{\pi}_1^{\mathrm{OD},1} \coloneqq \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0^{\perp}$ and $\boldsymbol{\pi}_1^{\mathrm{OD},2} \coloneqq \boldsymbol{\pi}_0^{\perp}\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0$ follow from the multiplication of $\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}_0^{\perp}$, respectively, once from each the left and the right. With $\boldsymbol{H}_0^{\perp} = \boldsymbol{H}_0\cdot\boldsymbol{\pi}_0^{\perp}$ and using that $\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}_0^{\perp}$ commute with $\boldsymbol{H}_0$ as operators on $\mathcal{H}_{\mathrm{f}}$, we obtain for the total off-diagonal operator $\boldsymbol{\pi}_1^{\mathrm{OD}} = \boldsymbol{\pi}_1^{\mathrm{OD},1} + \boldsymbol{\pi}_1^{\mathrm{OD},2}$,

$$\begin{aligned}\boldsymbol{\pi}_1^{\mathrm{OD}} &= \boldsymbol{\pi}_0\cdot\boldsymbol{b}_1\cdot\boldsymbol{\pi}_0^{\perp}\cdot(E_\nu\mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^{\perp})^{-1} \\ &\quad - (E_\nu\mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^{\perp})^{-1}\cdot\boldsymbol{\pi}_0^{\perp}\cdot\boldsymbol{b}_1\cdot\boldsymbol{\pi}_0 \\ &= \frac{i}{2}[\boldsymbol{\pi}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{H}_0 + E_\nu\mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}}\cdot(E_\nu\mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^{\perp})^{-1} \\ &\quad \cdot\boldsymbol{\pi}_0^{\perp} + (E_\nu\mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^{\perp})^{-1}\cdot\boldsymbol{\pi}_0^{\perp}\cdot\{\boldsymbol{H}_0 + E_\nu\mathbf{1}_{\mathrm{f}},\boldsymbol{\pi}_0\}_{\mathrm{s}}\cdot\boldsymbol{\pi}_0].\end{aligned} \tag{A14}$$

In order to evaluate $\boldsymbol{\pi}_1^{\mathrm{OD}}$ in terms of the connection coefficients, we recall that the Hamilton operator symbol can be written in its spectral form as

$$\boldsymbol{H}_0(q,p) = \sum_{n\in\mathbb{N}} E_n(q,p)\xi_n(q,p)\langle\xi_n(q,p),\cdot\rangle_{\mathrm{f}}, \tag{A15}$$

where $E_n(q,p)$ is the real-valued energy band function for the quantum number n. Consequently, derivations of $\boldsymbol{H}_0(q,p)$ with respect to q and p consist of three contributions for every n due to the product rule. This is for example relevant for the Poisson brackets that enter Eq. (A14). To illustrate the explicit evaluation of the respective terms, we compute the left contributions of the first term in $\boldsymbol{\pi}_1^{\mathrm{OD}}$, i.e.,

$$\begin{aligned}\boldsymbol{\pi}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{H}_0 + E_\nu\mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}} &= \boldsymbol{\pi}_0\cdot\left(\frac{\partial\boldsymbol{\pi}_0}{\partial q}\frac{\partial(\boldsymbol{H}_0 + E_\nu\mathbf{1}_{\mathrm{f}})}{\partial p} - \frac{\partial\boldsymbol{\pi}_0}{\partial p}\frac{\partial(\boldsymbol{H}_0 + E_\nu\mathbf{1}_{\mathrm{f}})}{\partial q}\right) \\ &= \xi_\nu\left\langle\frac{\partial\xi_\nu}{\partial q},\cdot\right\rangle_{\mathrm{f}}\sum_n\left(\frac{\partial(E_n + E_\nu)}{\partial p}\xi_n\langle\xi_n,\cdot\rangle_{\mathrm{f}} + E_n\left(\frac{\partial\xi_n}{\partial p}\langle\xi_n,\cdot\rangle_{\mathrm{f}} + \xi_n\left\langle\frac{\partial\xi_n}{\partial p},\cdot\right\rangle_{\mathrm{f}}\right)\right) \\ &\quad - \xi_\nu\left\langle\frac{\partial\xi_\nu}{\partial p},\cdot\right\rangle_{\mathrm{f}}\sum_n\left(\frac{\partial(E_n + E_\nu)}{\partial q}\xi_n\langle\xi_n,\cdot\rangle_{\mathrm{f}} + E_n\left(\frac{\partial\xi_n}{\partial q}\langle\xi_n,\cdot\rangle_{\mathrm{f}} + \xi_n\left\langle\frac{\partial\xi_n}{\partial q},\cdot\right\rangle_{\mathrm{f}}\right)\right).\end{aligned}$$

Then, let us replace the partial derivatives by their connection representatives and relabel certain indices in order to obtain the following result:

$$\boldsymbol{\pi}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{H}_0 + E_\nu\mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}} =: \sum_n \xi_\nu\langle\xi_n,\cdot\rangle_{\mathrm{f}}A_{\nu n}(q,p), \tag{A16}$$

where we defined the real-valued function $A_{\nu n}(q,p) \in C^\infty(\Gamma_s,\mathbb{R})$ according to

$$A_{\nu n} \coloneqq \left(\left(\mathcal{A}_{q\nu}{}^{n}\frac{\partial(E_n+E_\nu)}{\partial p} - \mathcal{A}_{p\nu}{}^{n}\frac{\partial(E_n+E_\nu)}{\partial q}\right) + (E_n-E_m)(\mathcal{A}_{p\nu}{}^{m}\mathcal{A}_{qm}{}^{n} - \mathcal{A}_{q\nu}{}^{m}\mathcal{A}_{pm}{}^{n})\right). \tag{A17}$$

Note that the quantum number ν is *fixed* while n and m run over all natural numbers. To obtain the first term of $\boldsymbol{\pi}_1^{\mathrm{OD}}$, we still need to multiply by the remaining factor $(E_\nu \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^\perp)^{-1}\cdot\boldsymbol{\pi}_0^\perp$ from the right which yields

$$\begin{aligned}&\frac{i}{2}\boldsymbol{\pi}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{H}_0+E_\nu\mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}}\cdot(E_\nu\mathbf{1}_{\mathrm{f}}-\boldsymbol{H}_0^\perp)^{-1}\cdot\boldsymbol{\pi}_0^\perp\\ &\quad=\frac{i}{2}\sum_n \xi_\nu\langle\xi_n,\cdot\rangle_{\mathrm{f}}A_{\nu n}(q,p)\cdot\sum_{l\neq\nu}\frac{\xi_l\langle\xi_l,\cdot\rangle_{\mathrm{f}}}{E_\nu-E_l}\\ &\quad=\frac{i}{2}\sum_{n\neq\nu}\frac{A_{\nu n}}{E_\nu-E_n}\xi_\nu\langle\xi_n,\cdot\rangle_{\mathrm{f}}.\end{aligned} \tag{A18}$$

Note that this operator has indeed only off-diagonal contributions as it projects on the state ξ_ν from any other state ξ_n, $n\neq\nu$. It is then easy to evaluate the remaining contribution to $\boldsymbol{\pi}_1^{\mathrm{OD}}$ without further calculations. According to the construction step (S1–2) the scheme requires that the projection symbol is self-adjoint $\boldsymbol{\pi}=\boldsymbol{\pi}^*$ such that the remaining contribution of $\boldsymbol{\pi}_1^{\mathrm{OD}}$ must evaluate to yield the total result

$$\boldsymbol{\pi}_1^{\mathrm{OD}} = \frac{i}{2}\sum_{n\neq\nu}\frac{A_{\nu n}}{E_\nu-E_n}(\xi_\nu\langle\xi_n,\cdot\rangle_{\mathrm{f}} - \xi_n\langle\xi_\nu,\cdot\rangle_{\mathrm{f}}). \tag{A19}$$

Thereby, note that any of the functions $A_{\nu n}$, E_n, and ξ_n are real valued. It is easy to check that indeed an explicit evaluation of the second summand in Eq. (A14) for $\boldsymbol{\pi}_1^{\mathrm{OD}}$ yields the same result. We have thus determined all contributions to $\boldsymbol{\pi}_{(1)}$. For closing this section, we emphasize that $\boldsymbol{\pi}_{(1)}(q,p)$ depends on the heavy phase space variables. Quantizing it with respect to the slow phase space variables yields a nontrivial operator with respect to the heavy subsystem and, hence, does not simplify the task to find (approximate) solutions for the quantum problem. The next step of the scheme consists in constructing a unitary symbol $\boldsymbol{u}$ which maps the dynamical subspace related to $\boldsymbol{\pi}_{(1)}$ to a suitable reference subspace $\mathcal{K}_{\mathrm{f}}\subset\mathcal{H}_{\mathrm{f}}$.

2. Construction of the Moyal unitary

We choose an arbitrary, but suitable, reference subspace $\mathcal{K}_{\mathrm{f}}\subset\mathcal{H}_{\mathrm{f}}$ by selecting one fixed set of values $(q_0,p_0)\in\Gamma_s$. We denote the eigenbasis of $\mathcal{H}_{\mathrm{f}}$ at (q_0,p_0) by $\{\xi_n(q_0,p_0)\}_{n\in\mathbb{N}} =: \{\zeta_n\}_{n\in\mathbb{N}}$ and define the reference projection as

$$\boldsymbol{\pi}_{\mathrm{p}} \coloneqq \xi_\nu(q_0,p_0)\langle\xi_\nu(q_0,p_0),\cdot\rangle_{\mathrm{f}} =: \zeta_\nu\langle\zeta_\nu,\cdot\rangle_{\mathrm{f}}. \tag{A20}$$

In order to mediate between $\mathcal{K}_{\mathrm{f}}$ and the subspace associated with $\boldsymbol{\pi}$, the scheme suggests to compute a unitary symbol $\boldsymbol{u}$ given as a formal power series in ε. We restrict the computation to the first order $\boldsymbol{u}_{(1)}=\boldsymbol{u}_0+\varepsilon\boldsymbol{u}_1$. It makes sense to choose

$$\boldsymbol{u}_0(q,p) \coloneqq \sum_{n\geq 0}\zeta_n\langle\xi_n(q,p),\cdot\rangle_{\mathrm{f}}, \tag{A21}$$

as initial data of the iteration. This is of course a choice which should be adapted to the physical situation at hand. The given option trivially satisfies the zeroth order of the space adiabatic scheme, namely

$$\begin{aligned}&(\mathrm{S2}-1)\ \boldsymbol{u}_0\cdot\boldsymbol{u}_0^* = \mathbf{1}_{\mathrm{f}}, \qquad (\mathrm{S2}-2)\ \boldsymbol{u}_0^*\cdot\boldsymbol{u}_0=\mathbf{1}_{\mathrm{f}},\\ &(\mathrm{S2}-3)\ \boldsymbol{u}_0\cdot\boldsymbol{\pi}_0\cdot\boldsymbol{u}_0^* = \boldsymbol{\pi}_{\mathrm{p}}.\end{aligned} \tag{A22}$$

In order to determine $\boldsymbol{u}_1$, it is useful to split it into a Hermitian and an anti-Hermitian part using the symbols $\boldsymbol{h}_1=\boldsymbol{h}_1^*$ and $\boldsymbol{k}_1=-\boldsymbol{k}_1^*$ such that $\boldsymbol{u}_{(1)} \coloneqq \boldsymbol{u}_0+\varepsilon(\boldsymbol{h}_1+\boldsymbol{k}_1)\cdot\boldsymbol{u}_0$.

a. Conditions (S2–1) and (S2–2): $\boldsymbol{u}\star_\varepsilon\boldsymbol{u}^*=\mathbf{1}_{\mathrm{f}}=\boldsymbol{u}^*\star_\varepsilon\boldsymbol{u}$

The unitarity conditions (S2–1) and (S2–2) yield the same results, and so we restrict our interest to the first condition. It evaluates in terms of $\boldsymbol{h}_1$ to the equation

$$\boldsymbol{u}_0\cdot\boldsymbol{u}_0^* - \mathbf{1}_{\mathrm{f}} + \varepsilon\left(\frac{i}{2}\{\boldsymbol{u}_0,\boldsymbol{u}_0^*\}_{\mathrm{s}} + 2\boldsymbol{h}_1\right) = \mathcal{O}_0(\varepsilon^2), \tag{A23}$$

and likewise for the second condition (S2–2). At zeroth order, the resulting conditions $\boldsymbol{u}_0\cdot\boldsymbol{u}_0^*-\mathbf{1}_{\mathrm{f}}=0$ and $\boldsymbol{u}_0^*\cdot\boldsymbol{u}_0-\mathbf{1}_{\mathrm{f}}=0$ are trivially satisfied for the choice of $\boldsymbol{u}_0$ in (A21). For the first order contribution, the scheme requires that the terms in the brackets vanish identically. This yields a determining equation for $\boldsymbol{h}_1$ for which we evaluate

$$\frac{\partial\boldsymbol{u}_0}{\partial\rho} = \sum_n\zeta_n\left\langle\frac{\partial\xi_n}{\partial\rho},\cdot\right\rangle_{\mathrm{f}} = \sum_n\mathcal{A}_{\rho n}{}^{m}\zeta_n\langle\xi_m,\rangle_{\mathrm{f}}, \tag{A24}$$

$$\frac{\partial\boldsymbol{u}_0^*}{\partial\rho} = \sum_n\frac{\partial\xi_n}{\partial\rho}\langle\zeta_n,\cdot\rangle_{\mathrm{f}} = \sum_n\mathcal{A}_{\rho n}{}^{m}\xi_m\langle\zeta_n,\cdot\rangle_{\mathrm{f}}. \tag{A25}$$

The total Hermitian part $\boldsymbol{u}_1^{\mathrm{h}} \coloneqq \boldsymbol{h}_1\cdot\boldsymbol{u}_0$ is then given according to Eq. (A23) by

$$\begin{aligned}\boldsymbol{u}_1^{\mathrm{h}} &= -\frac{i}{4}\{\boldsymbol{u}_0,\boldsymbol{u}_0^*\}_{\mathrm{s}}\cdot\boldsymbol{u}_0\\ &= \frac{i}{4}\sum_{n,m,k}(\mathcal{A}_{qn}{}^{m}\mathcal{A}_{pm}{}^{k} - \mathcal{A}_{pn}{}^{m}\mathcal{A}_{qm}{}^{k})\zeta_n\langle\xi_k,\cdot\rangle_{\mathrm{f}}.\end{aligned} \tag{A26}$$

The anti-Hermitian part $\boldsymbol{k}_1$ is determined by condition (S2–3).

b. Condition (S2–3): $\boldsymbol{u}\star_\varepsilon\boldsymbol{\pi}\star_\varepsilon\boldsymbol{u}^* = \boldsymbol{\pi}_{\mathrm{p}}$

We evaluate condition (S2–3) up to first order in the perturbations and obtain at zeroth order the obvious result $\boldsymbol{u}_0\cdot\boldsymbol{\pi}_0\cdot\boldsymbol{u}_0^* = \boldsymbol{\pi}_{\mathrm{p}}$. In order to determine the first order contributions and hence $\boldsymbol{k}_1$, we closely follow Teufel [[5], p. 86] and make the following definition:

$$\boldsymbol{w}_{(1)} \coloneqq \boldsymbol{u}_0 + \varepsilon\boldsymbol{h}_1\cdot\boldsymbol{u}_0 = \boldsymbol{u}_{(1)} - \varepsilon\boldsymbol{k}_1\cdot\boldsymbol{u}_0, \tag{A27}$$

which simply separates the Hermitian and the anti-Hermitian part of $\boldsymbol{u}_{(1)}$. Due to the conditions (S2–1) and (S2–2), we know that $\boldsymbol{w}_1$ satisfies $\boldsymbol{w}_{(1)}\star_\varepsilon\boldsymbol{w}^*_{(1)} = \mathbf{1}_{\mathrm{f}} + \mathcal{O}_0(\varepsilon^2)$, and $\boldsymbol{w}^*_{(1)}\star_\varepsilon\boldsymbol{w}_{(1)} = \mathbf{1}_{\mathrm{f}} + \mathcal{O}_0(\varepsilon^2)$. Let us then introduce a symbol function $\boldsymbol{K}_1$ to subsume the contributions in (S2–3) coming from the symbol $\boldsymbol{w}_{(1)}$ according to

$$\boldsymbol{w}_{(1)}\star_\varepsilon\boldsymbol{\pi}\star_\varepsilon\boldsymbol{w}^*_{(1)} - \boldsymbol{\pi}_{\mathrm{p}} =: \varepsilon\boldsymbol{K}_1 + \mathcal{O}_0(\varepsilon^2). \tag{A28}$$

With this definition, the evaluation of (S1–3) up to first order yields

$$\boldsymbol{u}_{(1)}\star_\varepsilon\boldsymbol{\pi}\star_\varepsilon\boldsymbol{u}^*_{(1)} - \boldsymbol{\pi}_{\mathrm{p}} =: \varepsilon(\boldsymbol{K}_1 + [\boldsymbol{k}_1,\boldsymbol{\pi}_{\mathrm{p}}]_{\mathrm{f}}) + \mathcal{O}_0(\varepsilon^2). \tag{A29}$$

The term in the round brackets must vanish to satisfy the requirements of SAPT. A possible solution to this is given by $\boldsymbol{k}_1 = [\boldsymbol{\pi}_{\mathrm{p}},\boldsymbol{K}_1]$ *if* $\boldsymbol{K}_1$ is Hermitian and off-diagonal with respect to $\boldsymbol{\pi}_{\mathrm{p}}$; namely we must ensure that

$$\boldsymbol{\pi}_{\mathrm{p}}\cdot\boldsymbol{K}_1\cdot\boldsymbol{\pi}_{\mathrm{p}} = 0 = \boldsymbol{\pi}_{\mathrm{p}}^{\perp}\cdot\boldsymbol{K}_1\cdot\boldsymbol{\pi}_{\mathrm{p}}^{\perp}. \tag{A30}$$

To show the second equality, we use that $\boldsymbol{w}_{(1)}$ satisfies (S1–1) and (S1–2) up to second order in the perturbations such that $\boldsymbol{\pi}_0^{\perp}$ can be written as

$$\begin{aligned}\mathbf{1}_{\mathrm{f}} - \boldsymbol{\pi}_{\mathrm{p}} &= \boldsymbol{w}_{(1)}\star_\varepsilon\boldsymbol{w}^*_{(1)} - \boldsymbol{\pi}_{\mathrm{p}} + \mathcal{O}_0(\varepsilon^2)\\ &= \boldsymbol{w}_{(1)}\star_\varepsilon\boldsymbol{w}^*_{(1)} + \boldsymbol{w}_{(1)}\star_\varepsilon\boldsymbol{\pi}\star_\varepsilon\boldsymbol{w}^*_{(1)} + \varepsilon\boldsymbol{K}_1 + \mathcal{O}_0(\varepsilon^2)\\ &= \boldsymbol{w}_{(1)}\star_\varepsilon(\mathbf{1}_{\mathrm{f}} - \boldsymbol{\pi})\star_\varepsilon\boldsymbol{w}^*_{(1)} + \varepsilon\boldsymbol{K}_1 + \mathcal{O}_0(\varepsilon^2).\end{aligned} \tag{A31}$$

We also recall the definition $\boldsymbol{K}_1 \coloneqq \varepsilon^{-1}(\boldsymbol{w}_{(1)}\star_\varepsilon\boldsymbol{\pi}\star_\varepsilon\boldsymbol{w}^*_{(1)} - \boldsymbol{\pi}_{\mathrm{p}}) + \mathcal{O}_0(\varepsilon^1)$ which underlines that $\boldsymbol{K}_1$ is the zeroth order symbol of the given expression. Besides, note that $\boldsymbol{\pi}$ as a Moyal projector satisfies the relation $\boldsymbol{\pi}\star_\varepsilon(\mathbf{1}_{\mathrm{f}} - \boldsymbol{\pi}) = 0$. Omitting any terms of higher than zeroth order in ε yields

$$\begin{aligned}\boldsymbol{\pi}_{\mathrm{p}}^{\perp}\cdot\boldsymbol{K}_1\cdot\boldsymbol{\pi}_{\mathrm{p}}^{\perp} &= \left[\frac{1}{\varepsilon}\boldsymbol{\pi}_{\mathrm{p}}^{\perp}\cdot(\boldsymbol{w}_{(1)}\star_\varepsilon\boldsymbol{\pi}\star_\varepsilon\boldsymbol{w}^*_{(1)} - \boldsymbol{\pi}_{\mathrm{p}})\cdot\boldsymbol{\pi}_{\mathrm{p}}^{\perp}\right]_0 = \left[\frac{1}{\varepsilon}\boldsymbol{\pi}_{\mathrm{p}}^{\perp}\star_\varepsilon\boldsymbol{w}_{(1)}\star_\varepsilon\boldsymbol{\pi}\star_\varepsilon\boldsymbol{w}^*_{(1)}\star_\varepsilon\boldsymbol{\pi}_{\mathrm{p}}^{\perp}\right]_0\\ &= \left[\frac{1}{\varepsilon}\boldsymbol{\pi}_{\mathrm{p}}^{\perp}\star_\varepsilon\boldsymbol{w}_{(1)}\star_\varepsilon\boldsymbol{\pi}\star_\varepsilon\boldsymbol{w}^*_{(1)}\star_\varepsilon(\boldsymbol{w}_{(1)}\star_\varepsilon(\mathbf{1}_{\mathrm{f}} - \boldsymbol{\pi})\star_\varepsilon\boldsymbol{w}^*_{(1)} + \varepsilon\boldsymbol{K}_1)\right]_0\\ &= \left[(\boldsymbol{w}_{(1)}\star_\varepsilon(\mathbf{1}_{\mathrm{f}} - \boldsymbol{\pi})\star_\varepsilon\boldsymbol{w}^*_{(1)} + \varepsilon\boldsymbol{K}_1)\star_\varepsilon\boldsymbol{w}_{(1)}\star_\varepsilon\boldsymbol{\pi}\star_\varepsilon\boldsymbol{w}^*_{(1)}\star_\varepsilon\boldsymbol{K}_1\right]_0\\ &= 0.\end{aligned} \tag{A32}$$

The very same reasoning leads to $\boldsymbol{\pi}_{\mathrm{p}}\cdot\boldsymbol{K}_1\cdot\boldsymbol{\pi}_{\mathrm{p}} = 0$. This shows that $\boldsymbol{K}_1$ contains indeed only an off-diagonal contribution and it is admissible to determine $\boldsymbol{k}_1$ according to $\boldsymbol{k}_1 = [\boldsymbol{\pi}_{\mathrm{p}},\boldsymbol{K}_1]$. According to (S2–3), we have that

$$\boldsymbol{K}_1 = \boldsymbol{h}_1\cdot\boldsymbol{\pi}_{\mathrm{p}} + \boldsymbol{\pi}_{\mathrm{p}}\cdot\boldsymbol{h}_1 + \boldsymbol{u}_0\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{u}_0^* + \frac{i}{2}\boldsymbol{u}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{u}_0^*\}_{\mathrm{s}} + \frac{i}{2}\{\boldsymbol{u}_0,\boldsymbol{u}_0^*\}_{\mathrm{s}}\cdot\boldsymbol{\pi}_{\mathrm{p}}. \tag{A33}$$

To simplify $[\boldsymbol{\pi}_{\mathrm{p}},\boldsymbol{K}_1]$, we use several identities. First, we employ $\boldsymbol{h}_1 = -(i/4)\{\boldsymbol{u}_0,\boldsymbol{u}_0^*\}_{\mathrm{s}}$ from above. We also use that

$$[\boldsymbol{\pi}_{\mathrm{p}},\boldsymbol{u}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{u}_0^*\}_{\mathrm{s}}]_{\mathrm{f}} = [\boldsymbol{\pi}_{\mathrm{p}},\{\boldsymbol{u}_0,\boldsymbol{u}_0^*\}_{\mathrm{s}}]_{\mathrm{f}}, \tag{A34}$$

which can easily be shown by using the Riesz representation of the symbols and the connection representation of their derivatives. In total, this yields for the anti-Hermitian part $\boldsymbol{u}_1^{\mathrm{ah}} \coloneqq \boldsymbol{k}_1\cdot\boldsymbol{u}_0$ of $\boldsymbol{u}_1$

$$\boldsymbol{u}_1^{\mathrm{ah}} = [\boldsymbol{\pi}_{\mathrm{p}},\boldsymbol{u}_0\cdot\boldsymbol{\pi}_1^{\mathrm{OD}}\cdot\boldsymbol{u}_0^*]_{\mathrm{f}}\cdot\boldsymbol{u}_0 + \frac{i}{4}[\boldsymbol{\pi}_{\mathrm{p}},\{\boldsymbol{u}_0,\boldsymbol{u}_0^*\}_{\mathrm{s}}]_{\mathrm{f}}\cdot\boldsymbol{u}_0. \tag{A35}$$

One could finally insert the formula for $\boldsymbol{\pi}_1^{\mathrm{OD}}$ that we already computed in order to express $\boldsymbol{u}_{(1)}$ by only zeroth order symbols.

3. Construction of the effective Hamiltonian

We construct $\boldsymbol{h}_{\mathrm{eff},(2)}$ iteratively by using the condition (S3), i.e., $\boldsymbol{h}_{\mathrm{eff}} \coloneqq \boldsymbol{u}\star_\varepsilon\boldsymbol{H}\star_\varepsilon\boldsymbol{u}^*$. Moreover, we project on the relevant energy band associated with $\boldsymbol{\pi}_{\mathrm{p}}$. The zeroth order contribution is of course trivial and yields

$$\boldsymbol{h}_{\mathrm{eff},0,\mathrm{p}} = \boldsymbol{\pi}_{\mathrm{p}}\cdot\boldsymbol{u}_0\cdot\boldsymbol{H}_0\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}} = \sum_n E_n(q,p)\zeta_n\langle\zeta_n,\cdot\rangle_{\mathrm{f}}. \tag{A36}$$

The quantization of this symbol with respect to the slow degrees of freedom yields the standard Born-Oppenheimer approximation. For the higher order contributions of $\boldsymbol{h}_{\mathrm{eff},(2),\mathrm{p}}$, the evaluation of the double star product would be cumbersome. It is therefore useful to star multiply (S3) by $\boldsymbol{u}$ from the right. For the first order effective Hamilton symbol this yields

$$\begin{aligned}\boldsymbol{u}\star_\varepsilon\boldsymbol{H}-\boldsymbol{h}_{\mathrm{eff},0}\star_\varepsilon\boldsymbol{u}&=\varepsilon\boldsymbol{h}_{\mathrm{eff},1}\star_\varepsilon\boldsymbol{u}+\mathcal{O}_0(\varepsilon^2)\\&=\varepsilon\boldsymbol{h}_{\mathrm{eff},1}\cdot\boldsymbol{u}_0+\mathcal{O}_0(\varepsilon^2).\end{aligned}\tag{A37}$$

The determining equation for $\boldsymbol{h}_{\mathrm{eff},1}$ is thus given by

$$\boldsymbol{h}_{\mathrm{eff},1}=\left[\boldsymbol{u}_1\cdot\boldsymbol{H}_0-\boldsymbol{h}_{\mathrm{eff},0}\cdot\boldsymbol{u}_1+\frac{i}{2}\{\boldsymbol{u}_0,\boldsymbol{H}_0\}_\mathrm{s}-\frac{i}{2}\{\boldsymbol{h}_{\mathrm{eff},0},\boldsymbol{u}_0\}_\mathrm{s}\right]\cdot\boldsymbol{u}_0^*.\tag{A38}$$

We desist from evaluating this expression further as we are mainly interested in the projection on the relevant energy band. In particular, we compute

$$\begin{aligned}\boldsymbol{h}_{\mathrm{eff},1,\mathrm{p}}&=\boldsymbol{\pi}_\mathrm{p}\cdot\boldsymbol{h}_{\mathrm{eff},1}\cdot\boldsymbol{\pi}_\mathrm{p}\\&=\boldsymbol{\pi}_\mathrm{p}\cdot\boldsymbol{u}_1\cdot(\boldsymbol{H}_0-E_\nu)\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_\mathrm{p}\\&\quad+\frac{i}{2}\boldsymbol{\pi}_\mathrm{p}\cdot\{\boldsymbol{u}_0,\boldsymbol{H}_0+E_\nu\mathbf{1}_\mathrm{f}\}_\mathrm{s}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_\mathrm{p}\\&=\frac{i}{2}\boldsymbol{\pi}_\mathrm{p}\cdot\{\boldsymbol{u}_0,\boldsymbol{H}_0+E_\nu\mathbf{1}_\mathrm{f}\}_\mathrm{s}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_\mathrm{p},\end{aligned}\tag{A39}$$

where the first two contributions cancel each other since $\boldsymbol{H}\cdot\boldsymbol{u}_0\cdot\boldsymbol{\pi}_\mathrm{p}=E_\nu\boldsymbol{u}_0\cdot\boldsymbol{\pi}_\mathrm{p}$. Using the connection representation, it is easy to show that also the remaining contributions vanish identically. Therefore, we consider the following identity:

$$\boldsymbol{\pi}_\mathrm{p}\cdot\frac{\partial\boldsymbol{u}_0}{\partial\rho}=\mathcal{A}^m_{\rho\nu}\zeta_\nu\langle\xi_m,\cdot\rangle_\mathrm{f}=\boldsymbol{u}_0\cdot\boldsymbol{\pi}_0\cdot\frac{\partial\boldsymbol{\pi}_0}{\partial\rho}.\tag{A40}$$

As a consequence, we can reformulate $\boldsymbol{h}_{\mathrm{eff},1,\mathrm{p}}$ such that it is possible to use the identities that we found for determining $\boldsymbol{\pi}_1^{\mathrm{OD}}$, in particular (A16) and the subsequent definition. This gives

$$\begin{aligned}\boldsymbol{h}_{\mathrm{eff},1,\mathrm{p}}&=\boldsymbol{u}_0\cdot\boldsymbol{\pi}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{H}_0+E_\nu\mathbf{1}_\mathrm{f}\}_\mathrm{s}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_\mathrm{p}\\&=\sum_n\zeta_\nu\langle\xi_n,\cdot\rangle_\mathrm{f}A_{\nu n}\xi_\nu\langle\zeta_\nu,\cdot\rangle_\mathrm{f}\\&=A_{\nu\nu}\zeta_\nu\langle\zeta_\nu,\cdot\rangle_\mathrm{f}=0.\end{aligned}\tag{A41}$$

The last equality follows because $A_{\nu n}$ has no diagonal contributions, simply because $\mathcal{A}_{\rho n}{}^m$ has none and because $\mathcal{A}^m_{\rho n}=-\mathcal{A}^n_{\rho m}$. The very same reasoning for determining $\boldsymbol{h}_{\mathrm{eff},1}$ applies for $\boldsymbol{h}_{\mathrm{eff},2}$, i.e., star-multiplying condition (S3) by $\boldsymbol{u}$ from the right yields

$$\begin{aligned}\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}=\boldsymbol{\pi}_\mathrm{p}\cdot\Big[&-\boldsymbol{h}_{\mathrm{eff},1}\cdot\boldsymbol{u}_1+\frac{i}{2}\{\boldsymbol{u}_1,\boldsymbol{H}_0\}_\mathrm{s}-\frac{i}{2}\{E_\nu,\boldsymbol{u}_1\}_\mathrm{s}\\&-\frac{i}{2}\{\boldsymbol{h}_{\mathrm{eff},1},\boldsymbol{u}_0\}_\mathrm{s}+[\boldsymbol{u}_0\star_\varepsilon\boldsymbol{H}_0]_2-[E_\nu\star_\varepsilon\boldsymbol{u}_0]_2\Big]\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_\mathrm{p},\end{aligned}\tag{A42}$$

where the brackets with index "2" select the contributions of second order in ε of the terms inside the brackets. The following discussion simplifies the individual terms, starting with the first contribution to $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}$ which vanishes identically. To see this, it suffices to consider the left-hand side $\boldsymbol{\pi}_\mathrm{p}\cdot\boldsymbol{h}_{\mathrm{eff},1,\mathrm{p}}$ in which we will employ the explicit expression for $\boldsymbol{u}_1$, namely

$$\begin{aligned}\boldsymbol{\pi}_\mathrm{p}\cdot\boldsymbol{h}_{\mathrm{eff},1,\mathrm{p}}&=\boldsymbol{\pi}_\mathrm{p}\cdot\boldsymbol{u}_1\cdot(\boldsymbol{H}_0-E_\nu\mathbf{1}_\mathrm{f})\cdot\boldsymbol{u}_0^*\\&\quad+\frac{i}{2}\boldsymbol{\pi}_\mathrm{p}\cdot\{\boldsymbol{u}_0,\boldsymbol{H}_0+E_\nu\mathbf{1}_\mathrm{f}\}_\mathrm{s}\cdot\boldsymbol{u}_0\\&=-\frac{i}{2}\boldsymbol{\pi}_\mathrm{p}\cdot\boldsymbol{u}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{H}_0+E_\nu\mathbf{1}_\mathrm{f}\}_\mathrm{s}\cdot(\mathbf{1}_\mathrm{f}-\boldsymbol{\pi}_0)\cdot\boldsymbol{u}_0^*\\&\quad+\frac{i}{2}\boldsymbol{\pi}_\mathrm{p}\cdot\{\boldsymbol{u}_0,\boldsymbol{H}_0+E_\nu\mathbf{1}_\mathrm{f}\}_\mathrm{s}\cdot\boldsymbol{u}_0^*\\&\quad-\frac{i}{4}\boldsymbol{\pi}_\mathrm{p}\cdot[\{\boldsymbol{u}_0,\boldsymbol{u}_0^*\}_\mathrm{s}-\boldsymbol{\pi}_\mathrm{p}\cdot\{\boldsymbol{u}_0,\boldsymbol{u}_0^*\}_\mathrm{s}\\&\quad+\{\boldsymbol{u}_0,\boldsymbol{u}_0^*\}_\mathrm{s}\cdot\boldsymbol{\pi}_\mathrm{p}]\cdot\boldsymbol{u}_0\cdot(\boldsymbol{H}_0-E_\nu\mathbf{1}_\mathrm{f})\cdot\boldsymbol{u}_0^*\\&=\frac{i}{2}\boldsymbol{\pi}_\mathrm{p}\cdot\{\boldsymbol{u}_0,\boldsymbol{H}_0+E_\nu\mathbf{1}_\mathrm{f}\}_\mathrm{s}\cdot\boldsymbol{\pi}_0\cdot\boldsymbol{u}_0^*=0.\end{aligned}\tag{A43}$$

The second line in this computation obviously yields the fourth line by comparing the terms. The third line vanishes because the first and the second terms cancel each other while we use for the last term that $\{\boldsymbol{u}_0,\boldsymbol{u}_0^*\}_\mathrm{s}$ has no diagonal contributions. The fourth line corresponds simply to the diagonal first order effective Hamiltonian $\boldsymbol{h}_{\mathrm{eff},1,\mathrm{p}}$, and we have already shown that this vanishes identically. The two following contributions can be merged into one term, and by pulling $\boldsymbol{\pi}_\mathrm{p}$ into the Poisson bracket, they yield

$$\begin{aligned}&\frac{i}{2}\{\boldsymbol{\pi}_\mathrm{p}\cdot\boldsymbol{u}_1,\boldsymbol{H}_0+E_\nu\mathbf{1}_\mathrm{f}\}_\mathrm{s}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_\mathrm{p}\\&\quad=\frac{1}{4}\{\{\boldsymbol{\pi}_\mathrm{p}\cdot\boldsymbol{u}_0,\boldsymbol{H}_0+E_\nu\mathbf{1}_\mathrm{f}\}_\mathrm{s}\cdot(\boldsymbol{H}_0-E_\nu\mathbf{1}_\mathrm{f})^{-1}\cdot\boldsymbol{\pi}_0^\perp,\boldsymbol{H}_0\\&\qquad+E_\nu\mathbf{1}_\mathrm{f}\}_\mathrm{s}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_\mathrm{p}.\end{aligned}\tag{A44}$$

In terms of the fast eigenstates and the connection coefficients it is given by

$$\frac{i}{2}\{\boldsymbol{\pi}_{\mathrm{p}}\cdot\boldsymbol{u}_1,\boldsymbol{H}_0+E_\nu\mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}}$$
$$=-\frac{1}{4}\sum_{n\neq\nu}\left[\frac{\partial}{\partial q}\left[\frac{A_{\nu n}}{E_\nu-E_n}\right](E_\nu-E_n)\mathcal{A}_{p\nu}{}^n\right.$$
$$\left.-2\frac{\partial E_\nu}{\partial p}\frac{A_{\nu n}\mathcal{A}_{q\nu}{}^n}{E_\nu-E_n}-A_{\nu n}\mathcal{A}_{qn}{}^m\mathcal{A}_{pm}{}^\nu\frac{E_\nu-E_m}{E_\nu-E_n}\right]$$
$$+\frac{1}{4}\sum_{n\neq\nu}[---\quad(p\leftrightarrow q)\quad--],\tag{A45}$$

where in the second line we add the terms of the first line with every occurrence of "q" replaced by "p," and vice versa. We emphasize the difference between the connection symbols $\mathcal{A}$ and the functions A which we used for expressing $\boldsymbol{\pi}_1$. The fourth contribution to $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}$ vanishes again trivially as it includes $\boldsymbol{\pi}_{\mathrm{p}}\cdot\boldsymbol{h}_{\mathrm{eff},1}$. The two remaining contributions involve the second order Moyal product and are given by

$$\boldsymbol{\pi}_{\mathrm{p}}\cdot[[\boldsymbol{u}_0\star_\varepsilon\boldsymbol{H}_0]_2-[E_\nu\star_\varepsilon\boldsymbol{u}_0]_2]\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}}$$
$$=\boldsymbol{\pi}_{\mathrm{p}}\cdot\left[-\frac{1}{8}\frac{\partial^2\boldsymbol{u}_0}{\partial q^2}\frac{\partial^2(\boldsymbol{H}_0-E_\nu)}{\partial p^2}+\frac{1}{4}\frac{\partial^2\boldsymbol{u}_0}{\partial p\partial q}\frac{\partial^2(\boldsymbol{H}_0-E_\nu)}{\partial q\partial p}\right.$$
$$\left.-\frac{1}{8}\frac{\partial^2\boldsymbol{u}_0}{\partial p^2}\frac{\partial^2(\boldsymbol{H}_0-E_\nu)}{\partial q^2}\right]\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}}.\tag{A46}$$

To represent these contributions in terms of the states and connection coefficients, we make the following definitions:

$$\boldsymbol{\pi}_{\mathrm{p}}\cdot\left[-\frac{1}{8}\frac{\partial^2\boldsymbol{u}_0}{\partial q^2}\frac{\partial^2(\boldsymbol{H}_0-E_\nu)}{\partial p^2}\right]\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}}=:B_{\mathrm{eff},1}(q,p)\boldsymbol{\pi}_{\mathrm{p}},\tag{A47}$$

$$\boldsymbol{\pi}_{\mathrm{p}}\cdot\left[\frac{1}{4}\frac{\partial^2\boldsymbol{u}_0}{\partial p\partial q}\frac{\partial^2(\boldsymbol{H}_0-E_\nu)}{\partial q\partial p}\right]\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}}=:B_{\mathrm{eff},2}(q,p)\boldsymbol{\pi}_{\mathrm{p}},\tag{A48}$$

and the functions $B_{\mathrm{eff},1}(q,p)$ and $B_{\mathrm{eff},2}(q,p)$ are then given according to

$$B_{\mathrm{eff},1}(q,p)=-\frac{1}{8}\left[2\frac{\partial(E_n-E_\nu)}{\partial p}\mathcal{A}_{pn}{}^\nu+(E_n-E_\nu)\frac{\partial\mathcal{A}_{pn}{}^\nu}{\partial p}\right.$$
$$\left.+(E_n-2E_m+E_\nu)\mathcal{A}_{pn}{}^m\mathcal{A}_{pm}{}^\nu\right]$$
$$\cdot\left[\frac{\partial\mathcal{A}_{q\nu}{}^n}{\partial q}+\mathcal{A}_{q\nu}{}^k\mathcal{A}_{qk}{}^n\right]\cdot\boldsymbol{\pi}_{\mathrm{p}},$$
$$B_{\mathrm{eff},2}(q,p)=\frac{1}{4}\left[\frac{\partial(E_n-E_\nu)}{\partial q}\mathcal{A}_{p\nu}{}^n+\frac{\partial(E_n-E_\nu)}{\partial p}\mathcal{A}_{q\nu}{}^n\right.$$
$$+(E_n-E_\nu)\frac{\partial\mathcal{A}_{q\nu}{}^n}{\partial p}+(E_m-E_\nu)\mathcal{A}_{q\nu}{}^m\mathcal{A}_{pm}{}^n$$
$$\left.+(E_m-E_n)\mathcal{A}_{p\nu}{}^m\mathcal{A}_{qm}{}^n\right]\left[\frac{\partial\mathcal{A}_{qn}{}^\nu}{\partial p}-\mathcal{A}_{pn}{}^k\mathcal{A}_{qk}{}^\nu\right].\tag{A49}$$

The total contribution coming from the second order components of the Moyal product in $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}$ has then the form

$$\boldsymbol{\pi}_{\mathrm{p}}\cdot[[\boldsymbol{u}_0\star_\varepsilon\boldsymbol{H}_0]_2-[E_\nu\star_\varepsilon\boldsymbol{u}_0]_2]\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}}$$
$$=[B_{\mathrm{eff},1}(q,p)+B_{\mathrm{eff},2}(q,p)+B_{\mathrm{eff},1}(p,q)]\cdot\boldsymbol{\pi}_{\mathrm{p}},$$

and we emphasize that the last term simply arises from the first term by interchanging any occurrence of q by p and vice versa. These contributions together with those in Eq. (A45) build then the total effective Hamiltonian symbol $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}(q,p)$.

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