Quantum cosmological backreactions. II. Purely homogeneous quantum cosmology

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In this second paper in a series of four, we continue with the program of incorporating backreaction among the homogeneous and between the homogeneous and inhomogeneous degrees of freedom in quantum cosmological perturbation theory. The purpose of the present paper is to illustrate the formalism of space adiabatic perturbation theory for two simple quantum mechanical models, and to prove that backreaction indeed leads to additional correction terms in effective Hamiltonians that one would otherwise neglect in a crude Born-Oppenheimer approximation. The first model consists of a harmonic oscillator coupled to an anharmonic oscillator. The second model describes the coupling between a scalar matter field and gravity restricted to the purely homogeneous and isotropic sector. These results have potential phenomenological consequences for quantum cosmological models.

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I. INTRODUCTION

In recent years, significant progress has been made in the field of cosmology thanks to major improvements in experimental precision [1] and theoretical modeling [2]. Because of the spatially nearly homogeneous and isotropic distribution of matter on large scales and of the cosmic microwave background radiation [3,4], it is possible to describe many phenomena with symmetry-reduced models of gravity and matter. The cosmological principle builds the basis of our current inflationary concordance ΛCDM model of the Universe [3,5–9]. Despite the many explanations that this standard model provides for understanding the early universe, important questions within the scheme remain unanswered, for example the present H_0 tension [10] (see also Refs. [11,12] pointing to a possible alleviation of the tension) and the dark sector [13,14].

From a theoretical perspective, the concordance model is built on the very well-tested foundations of classical Einstein general relativity, and on the quantum field theoretical Standard Model of particle physics. The incompatibility of their mathematical frameworks suggests to model the very early universe by a fundamental theory of quantum gravity [15,16]. While the construction of such a theory is a nontrivial endeavor, there are several possible candidates for a theory of quantum gravity (see Ref. [17] for an extensive overview).

Now, there is hope that the above-mentioned advent of cosmological measurements could serve to falsify such quantum gravity theories. One advantage is that the cosmological principle suggests to split cosmological fields into a symmetry-reduced background and perturbations thereof. In the series of papers, of which this is the second one, we therefore build on the idea that a split into homogeneous and inhomogeneous modes at the classical level is meaningful.

In order to incorporate the ideas of quantum gravity, both the symmetry-reduced sector as well as the inhomogeneities should be subject to quantization. This procedure is inspired by the hybrid approach [18,19] to quantum cosmology in which the inhomogeneous degrees of freedom can be quantized by using the powerful machinery of quantum field theory on curved spacetimes (QFT on CST) [20].

Now, there are several problems regarding the formulation of such quantum cosmological perturbation theories. First, in order to use the machinery of QFT on CST, we need as an input a *classical* metric on which the quantum fields propagate. That metric is, however, *fundamentally quantum*. The framework which we employ in order to overcome these problems is similar to the one used in quantum fields in noncommutative spacetimes [21,22] and is denoted as space adiabatic perturbation theory (SAPT) [23]. If at least two different energy scales can be identified, such a quantization scheme comes automatically accompanied by a corresponding perturbation expansion with respect to the ratio of the

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gravitational coupling constant $\kappa := 8\pi G$ where G is Newton's constant, and the standard model matter coupling constant λ.

The second important problem of inhomogeneous quantum cosmology concerns the faithful consideration of interactions between the homogeneous and the perturbative sector. The difficulties are due to the nonlinear character of Einstein's equations, as well as the general difficulty of modeling coupled quantum systems. While there has been seminal progress in studying the evolution of quantum fields on effective classical backgrounds (see our references in [24]), the question of backreaction from the perturbations onto the homogeneous degrees of freedom has not been studied in great detail and by using rigorous perturbation schemes.

However, the quantum fluctuations of all degrees of freedom including the homogeneous ones are expected to be very strong during the Planck era. Thus, it is unclear whether semiclassical approximations of the fluctuations are sufficiently accurate [25–29].

SAPT provides just that—a rigorous formalism to incorporate backreaction. More precisely, it provides a perturbative scheme for deriving approximate quantum equations of motion for coupled quantum systems [30]. In our case, and in particular in the third and the fourth papers of this series [31,32], this allows us to analyze the quantum backreaction of the inhomogeneous cosmological fields on the homogeneous and dynamical quantum degrees of freedom.

For this purpose, SAPT uses the quasiadiabatic behavior of the system in the sense that one can separate a "fast" subsystem which provides energetic subspaces that are almost invariant under the dynamics of the full Hamilton constraint or operator $\hat{\boldsymbol{H}}$. It provides an iterative scheme to compute projection operators associated with these fast energy bands which commute with $\hat{\boldsymbol{H}}$ up to the desired order in ε. Eventually, the theory suggests to project onto one of these subspaces of the fast subsystem in order to obtain an effective Hamiltonian for the slow system only. Solving this Hamiltonian provides an approximate solution of the full problem. The well-known Born-Oppenheimer approximation for molecules corresponds precisely to the zeroth order of this scheme: There, the small mass ratio of electron and nuclei masses $\varepsilon^2 := m_e/M_n$ suggests to project the system onto one of the electron subspaces which are almost invariant under the dynamics of the full Hamiltonian (for a limited range of time). The scheme provides an effective backreaction term for the nuclei problem.

The Born-Oppenheimer approximation has already been applied to different models of quantum gravity [33–35]. Unfortunately, the formalism only applies to a certain class of problems (in particular, it does *not* apply to gauge-invariant quantum cosmological perturbation theory) and restricts to first order perturbation theory. SAPT extends the formalism accordingly. In [36–38], SAPT was first applied to quantum gravity. It was pointed out that SAPT, designed for quantum systems with finitely many degrees of freedom, needs to meet certain conditions in order to apply to QFT. These conditions, specifically certain Hilbert-Schmidt requirements, are not automatically met in inhomogeneous quantum cosmology [36–38].

In our exposition of SAPT for quantum cosmology, we aim at improving this situation. We apply SAPT to (perturbative) cosmological models in order to keep track of the backreactions between the homogeneous and inhomogeneous degrees of freedom. The first paper [24] of our series of four papers lays out the corresponding general theory. In particular, we include a self-contained introduction both to SAPT as well as to the relevant aspects of gauge-invariant cosmological perturbation theory. Besides, we discuss the challenges that occur when applying SAPT to a QFT in great detail.

In the present second paper, we apply the formalism of [24] to two quantum mechanical models. The first model is a fast harmonic oscillator coupled to a slow anharmonic one. It prepares our application of SAPT to the second model which is general relativity coupled to a Klein-Gordon field and then truncated to the purely homogeneous and isotropic degrees of freedom. In suitable variables and in the presence of a positive (negative) cosmological constant, this model can be considered as a fast harmonic oscillator coupled to a slow inverse (negative energy) harmonic oscillator; that is, the kinetic term has a sign opposite to that of a harmonic oscillator.

The purpose of these two models is twofold: On the one hand, it illustrates the space adiabatic formalism in a relatively simple and familiar context. On the other hand, we showcase how the formalism extracts very efficiently an effective Hamiltonian for the slow sector while incorporating the interaction with the fast one. In particular, it displays the backreaction between the two kinds of degrees of freedom. The second model should be considered as the purely homogeneous truncation of the quantum field theoretic models that we treat in the two subsequent papers [31,32].

The architecture of this paper is then as follows: In the next section, we briefly present the SAPT scheme and the conditions that have to be met for the theory to be applicable. For further details, we refer to the companion paper [24]. In Sec. III, we apply SAPT to the system of two coupled quantum oscillators. In addition to extracting the adiabatic corrections, we perform a spectral analysis of the effective Hamiltonian and combine the adiabatic expansion with the framework of quantum mechanical stationary perturbation theory [39,40]. In Sec. IV, we consider the second model with the same methods. As the spectrum is not pure point when the cosmological constant is positive, one cannot resort to stationary perturbation theory [41] but must use independent methods [42] for the spectral analysis of the effective Hamiltonian constraint. The pure point nature of the spectrum will lead to delicate matching conditions which

critically influence the size and structure of the kernel. Finally, in Sec. V, we summarize our findings and conclude.

II. SPACE ADIABATIC PERTURBATION THEORY

A. A brief overview of the basics

SAPT establishes approximate quantum equations of motion for coupled quantum systems whose exact solutions are not available. An important prerequisite for the theory is the identification of a perturbative parameter which compares two energy scales within the model. The two energy scales are related to two (or more) subsystems, one of which has a correspondingly high rate of change (the "fast" subsystem) compared to the other subsystem (the "slow" subsystem). The core of the approximation scheme relies on the space adiabatic theorem [23]. Therefore, let $\hat{\boldsymbol{H}} \in \mathcal{B}(\mathcal{H})$ be an (essentially) self-adjoint, bounded, Weyl-quantized Hamilton operator on the Hilbert space $\mathcal{H}$. The space adiabatic theorem states that there exists (under certain conditions to which we will come in Sec. II B) an orthogonal projection operator $\hat{\boldsymbol{\Pi}} \in \mathcal{B}(\mathcal{H})$ such that [30]

$$[\hat{\boldsymbol{H}}, \hat{\boldsymbol{\Pi}}] = \mathcal{O}_0(\varepsilon^\infty). \tag{1}$$

The estimate on the right-hand side means that for all $m \in \mathbb{N}$, there exists a constant $C_m \geq 0$ such that $\|[\hat{\boldsymbol{H}}, \hat{\boldsymbol{\Pi}}]\|_{\mathcal{B}(\mathcal{H})} \leq C_m \varepsilon^m$. As a result, it is possible to construct a projection operator which commutes in norm up to infinite order in ε with the full Hamilton operator and hence is almost invariant under its dynamics.

The starting point and the basic idea of the space adiabatic scheme consists in iteratively constructing such a projection operator. As it turns out, the projection operator is directly linked to one or several quantum number(s) of the fast subsystem. In particular, it is possible to extract quantum solutions of the fast system if we formally "fix" the heavy subsystem in the first step. The purpose of this analysis is twofold: On the one hand, these states already represent one part of the solution. On the other hand, they allow one to consider the effects of the fast subspaces on the slow subsystem *separately* for each subspace. In this sense, the scheme provides a perturbative decoupling of subspaces of the fast state space. Then, projecting onto one of these fast subspaces eventually allows one to define an "effective" Hamilton constraint or operator $\hat{\boldsymbol{h}}_{\text{eff}}$ which acts trivially on the fast subsystem. Thus, $\hat{\boldsymbol{h}}_{\text{eff}}$ provides an equation of motion or constraint for the slow subsystem only, which is relatively easy to solve. Moreover, it can be shown that the dynamics that it generates in case of a true Hamilton operator and regarding a time parameter t is identical to the original dynamics up to errors of order $\varepsilon^\infty|t|$ in the estimate from above [23,24].

Since all parts of the system are considered to be fundamentally quantum, let us start with a Hilbert space that splits into the tensor product $\mathcal{H} = \mathcal{H}_{\text{s}} \otimes \mathcal{H}_{\text{f}}$, where the labels "s" and "f" stand for slow and fast. Quantization with respect to the slow subsystem is indicated by hats, while quantum operators of the fast subsystem are given by bold letters. The canonical variables of the slow and the fast subsystems will be denoted by (q, P) and (x, y), respectively. The concrete realization of the scheme requires us, however, to represent the quantum theory of the adiabatically slow subsystem as a deformation or phase space quantization [43,44] (see Refs. [45,46] for recent reviews). This consists in assigning a quantum "symbol" function on the slow phase space Γ_{s} to its classical analog, instead of associating an operator $\hat{g}$ on some domain $\mathcal{D}_g \subset \mathcal{H}_{\text{s}}$ with each classical function (or distribution) on Γ_{s}. At the same time, we stick to the standard representation of quantum theory of the fast subsystem and display observables as operators on the Hilbert space $\mathcal{H}_{\text{f}}$. For the coupled system, operators consequently have the form of functions on the heavy phase space Γ_{s} with values in the bounded operators on $\mathcal{H}_{\text{f}}$, for example $\boldsymbol{B}(q, p) \in C^\infty(\Gamma_{\text{s}}, \mathcal{B}(\mathcal{H}_{\text{f}}))$.

These symbol functions play a crucial role in the definition of the subsequent quantum theory and only a certain class of symbol functions will eventually lead to a well-defined theory, motivated by the pseudodifferential calculus [47–51]. We note that the calculus automatically provides a perturbative scheme if we rescale the momentum variable P, subject to the phase space quantum theory, by a factor ε, i.e., $p := \varepsilon P$ [23]. In the following, this rescaling will implicitly be assumed.

As a starting point, we remark that the connection of phase space quantum mechanics with the conventional representation of quantum operators as continuous linear maps on a Hilbert space is given by the Schwartz kernel theorem. Its generalization to the coupled systems states that any (bounded operator)-valued phase space distribution $\boldsymbol{B}(q, p) \in \mathcal{S}'(\Gamma_{\text{s}}, \mathcal{B}(\mathcal{H}_{\text{f}}))$, i.e., the operator in the employed phase space representation, is uniquely associated with a linear operator $\hat{\boldsymbol{B}}: \mathcal{S}(\mathcal{C}_{\text{s}}, \mathcal{H}_{\text{f}}) \to \mathcal{S}'(\mathcal{C}_{\text{s}}, \mathcal{H}_{\text{f}})$ which corresponds to the operator in the standard tensor product form. Here, $\mathcal{C}_{\text{s}}$ is the configuration space of the slow subsystem. In particular, $\boldsymbol{B}(q, p)$ defines the integral kernel $\boldsymbol{K}_{\boldsymbol{B}}$ associated with the map $\hat{\boldsymbol{B}}$. For a Weyl ordering of operators and for some $\psi \in \mathcal{S}(\mathcal{C}_{\text{s}}, \mathcal{H}_{\text{f}})$, the quantum operator $\hat{\boldsymbol{B}}$ associated with its half-classical counterpart $\boldsymbol{B}$ is then given by [30]

$$(\hat{\boldsymbol{B}}\psi)(q, x) = \frac{1}{2\pi\varepsilon} \int\!\!\int_{\mathbb{R}^2} \boldsymbol{B}\left(\frac{1}{2}(q + \tilde{q}), p\right) e^{i\frac{p}{\varepsilon}(q-\tilde{q})} \psi(\tilde{q}, x) \mathrm{d}p \mathrm{d}\tilde{q} \in \mathcal{S}'(\mathcal{C}_{\text{s}}, \mathcal{H}_{\text{f}}). \tag{2}$$

In order to work with operators for which the above integral is uniformely convergent and such that Schwartz functions are mapped on Schwartz functions, we need to restrict our attention to a smaller class of observables than the tempered distributions, $\mathcal{S}'(\Gamma_s, \mathcal{B}(\mathcal{H}_f))$ [30]. Specifically, we use the class of operator–valued functions $S^m_\rho(\Gamma_s, \mathcal{B}(\mathcal{H}_f)) =: S^m_\rho$ for which $m \in \mathbb{R}$ and $0 \leq \rho \leq 1$. A phase space function $\boldsymbol{B}(q,p)$ belongs to S^m_ρ and is denoted as a "symbol" of class (m,ρ), if for every $\alpha, \beta \in \mathbb{N}$ there exists a positive constant $C_{\alpha,\beta}$ such that [30]

$$\sup_{q\in\mathbb{R}} \|(\partial_q^\alpha \partial_p^\beta \boldsymbol{B})(q,p)\|_{\mathcal{B}(\mathcal{H}_f)} \leq C_{\alpha,\beta} \langle p \rangle^{m-\rho|\beta|}, \tag{3}$$

for every $p \in \mathbb{R}$, where $\langle p \rangle = (1+p^2)^{\frac{1}{2}}$. Note that these symbols must be bounded functions with respect to q, but may grow polynomially with respect to p. Working with these symbol classes has the advantage that the symbols can be composed with one another, and adjoints as well as transposed operators can be well defined. In particular, the operator product carries over to the space of symbol functions and yields the continuous "star" or "Moyal" product [46,52,53] on this space. It is the pullback of the operator product on $\mathcal{H}_s$ to the Poisson algebra of phase space functions with values in the space of linear operators on $\mathcal{H}_f$. The product is an asymptotic expansion in ε and establishes the perturbative character of the space adiabatic theory. Let therefore be $\boldsymbol{B} \in S^{m_1}_\rho$ and $\boldsymbol{C} \in S^{m_2}_\rho$. Then, the operator product $\hat{\boldsymbol{B}}\hat{\boldsymbol{C}}$ yields a well-defined operator $\hat{\boldsymbol{D}}$ with symbol $\boldsymbol{D} \in S^{m_1+m_2}_\rho$ given by [30]

$$\boldsymbol{D}(q,p) = \sum_{k=0}^{\infty} \frac{(\frac{i\varepsilon}{2})^k}{k!} (\partial_q \partial_\xi - \partial_\rho \partial_p)^k \boldsymbol{B}(q,p) \cdot \boldsymbol{C}(\rho,\xi)|_{\rho=q,\xi=p} =: (\boldsymbol{B} \star_\varepsilon \boldsymbol{C})(q,p). \tag{4}$$

Here, we denote the operator product for operators acting on states in $\mathcal{H}_f$ with a dot "$\cdot$." The construction scheme of SAPT and the conditions on the system can be stated as follows:

B. System requirements

The subsequent presentation of the scheme and the conditions that the system has to meet is based on the work by Panati *et al.* [23,30]. These conditions are quite restrictive and narrowly defined, thus excluding a variety of systems. For example, the unbounded Hamilton operator of the oscillator subsystem [cf. Eq. (12)] would not satisfy the conditions without some technical modifications. These modifications will be presented in the sequel. The conditions given in [23,30] split into four categories:

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

$$\mathcal{H} = L^2(\mathbb{R}) \otimes \mathcal{H}_f = L^2(\mathbb{R}, \mathcal{H}_f), \tag{5}$$

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

(C2) *The Hamilton operator* $\hat{\boldsymbol{H}}$ is the Weyl quantization of a symbol function $\boldsymbol{H}(q,p)$ in the symbol class $S^m_\rho(\Gamma_s, \mathcal{B}(\mathcal{H}_f))$. The Weyl quantization refers to the slow subsystem, and the function $\boldsymbol{H}(q,p)$ has values in the space of bounded self-adjoint operators on $\mathcal{H}_f$.

$(C3)_\gamma$ *Gap condition*. For any fixed $(q,p) \in \mathbb{R}^2$, the spectrum $\sigma(q,p)$ of the function $\boldsymbol{H}(q,p)$ contains at least one isolated subset, $\sigma_\nu(q,p)$, associated with (a) fixed quantum number(s) $\nu \in \mathbb{N}$ which is uniformly separated from the remainder $\sigma_{\text{rem}}(q,p) \coloneqq \sigma(q,p) \backslash \sigma_\nu(q,p)$. In particular, the minimal distance between the elements of $\sigma_\nu(q,p)$ and the remainder of the spectrum $\sigma_{\text{rem}}(q,p)$ is nonzero for every single $(q,p) \in \mathbb{R}^2$. More precisely, we can define two continuous "enclosing" functions, $f_\pm : \mathbb{R}^2 \to \mathbb{R}$ with $f_- \leq f_+$, such that

(G1) For every $(q,p) \in \mathbb{R}^2$, the spectral component $\sigma_\nu(q,p)$ is entirely contained in the interval $I(q,p) \coloneqq [f_-(q,p), f_+(q,p)]$.

(G2) The distance between the remainder $\sigma_{\text{rem}}(q,p)$ and the interval $I(q,p)$ is uniformly bounded away from zero, i.e., $\text{dist}[\sigma_{\text{rem}}(q,p), I(q,p)] \geq C_g \langle p \rangle^\gamma$.

(G3) The width of $I(z)$ is uniformly bounded: $\sup_{(q,p)\in\mathbb{R}^2} |f_+(q,p) - f_-(q,p)| \leq C_w < \infty$.

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

C. Manual of the adiabatic perturbation scheme

Given the prerequisites of the previous section, Sec. II B, the scheme of SAPT divides into three steps and relies on the existence of the three following symbol functions. Given the Hamilton symbol $\boldsymbol{H} \in S^m_\rho$, SAPT assures that [23]

(S1) there exists a unique formal symbol $\boldsymbol{\pi} = \sum_{i\geq 0} \varepsilon^i \boldsymbol{\pi}_i$ with $\boldsymbol{\pi}_i \in S^{-i\rho}_\rho(\mathcal{B}(\mathcal{H}_f))$ such that $\boldsymbol{\pi}_0$ is the spectral projection of $\boldsymbol{H}(q,p)$ corresponding to $\sigma_\nu(q,p)$ and with the properties

(S1–1) $\boldsymbol{\pi}\star_\varepsilon\boldsymbol{\pi}=\boldsymbol{\pi}$, (S1–2) $\boldsymbol{\pi}^*=\boldsymbol{\pi}$,
(S1–3) $\boldsymbol{H}\star_\varepsilon\boldsymbol{\pi}-\boldsymbol{\pi}\star_\varepsilon\boldsymbol{H}=0$.

It can be shown that the Weyl quantization of a resummation of $\boldsymbol{\pi}$ which we denote by $\boldsymbol{\pi}_\varepsilon$ is $\mathcal{O}_0(\varepsilon^\infty)$—close to an operator $\hat{\mathbf{\Pi}}$, i.e., $\hat{\mathbf{\Pi}}=\hat{\boldsymbol{\pi}}_\varepsilon+\mathcal{O}_0(\varepsilon^\infty)$ and $[\hat{\boldsymbol{H}},\hat{\mathbf{\Pi}}]=\mathcal{O}_0(\varepsilon^\infty)$ [[30] p. 75]. Hence, the symbol function $\boldsymbol{\pi}$ gives indeed a raise to an (almost) projector onto one of the dynamical subspaces of $\hat{\boldsymbol{H}}$.

(S2) Let $\boldsymbol{\pi}_\mathrm{p}$ be the projection on some "reference" subspace $\mathcal{K}_\mathrm{f}\subset\mathcal{H}_\mathrm{f}$. We assume that there exists a symbol $\boldsymbol{u}_0\in S^0_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ such that $\boldsymbol{u}_0\cdot\boldsymbol{\pi}_0\cdot\boldsymbol{u}_0^*=\boldsymbol{\pi}_\mathrm{p}$. Then, there is a formal symbol $\boldsymbol{u}=\sum_{i\geq0}\varepsilon^i\boldsymbol{u}_i$ with $\boldsymbol{u}_i\in S^{-i\rho}_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ such that

(S2–1) $\boldsymbol{u}^*\star_\varepsilon\boldsymbol{u}=\mathbf{1}_\mathrm{f}$, (S2–2) $\boldsymbol{u}\star_\varepsilon\boldsymbol{u}^*=\mathbf{1}_\mathrm{f}$,
(S2–3) $\boldsymbol{u}\star_\varepsilon\boldsymbol{\pi}\star_\varepsilon\boldsymbol{u}^*=\boldsymbol{\pi}_\mathrm{p}$.

The Weyl quantization of a resummation of $\boldsymbol{u}$ which we denote by $\boldsymbol{u}_\varepsilon$ gives rise to an operator $\hat{\boldsymbol{U}}=\hat{\boldsymbol{u}}_\varepsilon+\mathcal{O}_0(\varepsilon^\infty)$ for which it holds true that $\hat{\boldsymbol{U}}\,\hat{\mathbf{\Pi}}\,\hat{\boldsymbol{U}}=\hat{\boldsymbol{\pi}}_\mathrm{p}$ [[30], p. 85].

(S3) We construct a formal "effective" Hamilton symbol $\boldsymbol{h}_\mathrm{eff}=\sum_{i\geq0}\varepsilon^i\boldsymbol{h}_{\mathrm{eff},i}$ by means of

$$\boldsymbol{h}_\mathrm{eff}:=\boldsymbol{u}\star_\varepsilon\boldsymbol{H}\star_\varepsilon\boldsymbol{u}^*.$$

It is then true for systems with an external time parameter t and the Weyl quantizations $\hat{\boldsymbol{u}}$ and $\hat{\boldsymbol{h}}_\mathrm{eff}$ that [[30], p. 90]

$$e^{-i\hat{\boldsymbol{H}}t}-\hat{\boldsymbol{u}}^*e^{-i\hat{\boldsymbol{h}}_\mathrm{eff}t}\hat{\boldsymbol{u}}=\mathcal{O}_0(\varepsilon^\infty|t|). \tag{6}$$

Hence, after unitarily transforming back to the original Hilbert space, the dynamics generated by $\hat{\boldsymbol{h}}_\mathrm{eff}$ corresponds to the dynamics of the true Hamiltonian $\hat{\boldsymbol{H}}$ up to errors of order $\varepsilon^\infty|t|$.

Eventually, the aim is to compute the series expansion of $\boldsymbol{h}_\mathrm{eff}$ up to the desired order $I\in\mathbb{N}$ in ε, such that the above assertion about the dynamics is true up to errors of the order $\varepsilon^{I+1}|t|$. We emphasize that the perturbative development of the star product provides the possibility to iteratively determine $\boldsymbol{\pi}_{(I)}:=\sum_{i\leq I}\varepsilon^i\boldsymbol{\pi}_i$, $\boldsymbol{u}_{(I)}:=\sum_{i\leq I}\varepsilon^i\boldsymbol{u}_i$. In this work, we compute $\boldsymbol{\pi}_{(1)}$, $\boldsymbol{u}_{(1)}$, and $\boldsymbol{h}_{\mathrm{eff},(2)}$ for the oscillator and the cosmological models.

III. THE SHOWCASE EXAMPLE: COUPLED OSCILLATORS

A. Presentation of the system and preparations

We apply the space adiabatic perturbation scheme to a quantum system which comprises two coupled subsystems: An anharmonic oscillator, which can be identified with a heavy mass $M\in\mathbb{R}^+$, and a harmonic oscillator associated with a lighter mass $m\in\mathbb{R}^+$. We require the mass ratio $\varepsilon^2:=\frac{m}{M}$ to be small in order to demonstrate the space adiabatic formalism. Accordingly, the anharmonic oscillator with mass M admits a much smaller rate of change than the harmonic oscillator with mass m. The constant number ε serves as the perturbation parameter for the theory. In the following, we refer to the heavy anharmonic subsystem with phase space variables $(q,P)\in\Gamma_\mathrm{s}=\mathbb{R}^2$, while for the light harmonic oscillator we introduce the phase space variables $(x,y)\in\Gamma_\mathrm{f}=\mathbb{R}^2$. The classical Hamiltonian associated with the model is given as the four-times differentiable function on the Cartesian product of phase spaces $\Gamma_\mathrm{s}\times\Gamma_\mathrm{f}$,

$$H(q,P,x,y)=\frac{P^2}{2M}+\frac{y^2}{2m}+\frac{1}{2}m\omega(q)^2\cdot x^2\in C^4(\Gamma_\mathrm{s}\times\Gamma_\mathrm{f},\mathbb{R}), \tag{7}$$

where we have introduced the function

$$\omega(q):=\omega_0\left(1+\frac{q^2}{L^2}\right)\in C^2(\Gamma_\mathrm{s},\mathbb{R}^+). \tag{8}$$

The function ω mediates the coupling between the two oscillators and can be understood as a q-dependent frequency of the light, harmonic oscillator. The parameter $L\in\mathbb{R}^+$ has the dimension of a length and plays the role of a coupling constant between the subsystems. The coupling vanishes in the limit $L\to\infty$.

We quantize the system and start by considering the light harmonic oscillator. We specify the state space as a standard L^2-space and denote it as $L^2_\mathrm{f}(\mathbb{R})$. The quantum operators of the canonical variables x and y will be indicated by bold letters and shall act on the vectors in the Schwartz space $\mathcal{S}$ in the standard way. They satisfy the formal commutation relation

$$[\boldsymbol{x},\boldsymbol{y}]_\mathrm{f}=i\mathbf{1}_\mathrm{f}, \tag{9}$$

where we set $\hbar\equiv1$. Since the classical Hamilton function $H(q,P,x,y)$ does not contain any mixed products of the canonical variables x and y, there is no ordering choice to be made for the quantum theory. For the heavy, anharmonic oscillator, we take another L^2-space as the space of quantum states, and we denote it as $L^2_\mathrm{s}(\mathbb{R})$. The quantum operators of the canonical variables q and P will be indicated by hats and shall act in the known way, analogously to the light

oscillator. In order to make SAPT work at the technical level, we introduce a rescaled momentum operator $\hat{p} \coloneqq \varepsilon\hat{P}$. Hence, the standard commutation relation of position and momentum operator becomes

$$[\hat{q}, \hat{p}]_{\mathrm{s}} = i\varepsilon\hat{1}_{\mathrm{s}}. \tag{10}$$

Since the ordering of position and momentum operators plays a role for the heavy oscillator, we choose the Weyl ordering prescription of quantum operators [54,55]. The quantum theory of the coupled system has the tensor product Hilbert space

$$\mathcal{H} = L^2_{\mathrm{s}}(\mathbb{R}) \otimes L^2_{\mathrm{f}}(\mathbb{R}) \cong L^2(\mathbb{R}\times\mathbb{R}) \tag{11}$$

as its state space. Here, "$\otimes$" denotes the topological tensor product of Hilbert spaces.

Accordingly, we can define quantum operators by means of the topological tensor product of bounded operators on $\mathcal{H}$. These have the form $\hat{A}\otimes\boldsymbol{B} \in \mathcal{B}(L^2_{\mathrm{s}}(\mathbb{R}))\otimes\mathcal{B}(L^2_{\mathrm{f}}(\mathbb{R}))$ for $\hat{A}\in\mathcal{B}(L^2_{\mathrm{s}}(\mathbb{R}))$ and $\boldsymbol{B}\in\mathcal{B}(L^2_{\mathrm{f}}(\mathbb{R}))$. In a similar manner, we define the Hamilton operator $\hat{\boldsymbol{H}}$ associated with the classical Hamilton function H as a sum of tensor product operators,

$$\hat{\boldsymbol{H}} = \frac{\hat{P}^2}{2M}\otimes\mathbf{1}_{\mathrm{f}} + \hat{1}_{\mathrm{s}}\otimes\frac{\boldsymbol{y}^2}{2m} + \frac{1}{2}m\omega(\hat{q})^2\otimes\boldsymbol{x}^2. \tag{12}$$

Note that $\hat{\boldsymbol{H}}$ is *not* a bounded operator on the state space $\mathcal{H}$, but it is a well-defined, bounded operator on $C^\infty_{\mathrm{c}}(\mathbb{R})\otimes C^\infty_{\mathrm{c}}(\mathbb{R})$, i.e., on the topological tensor product of the spaces of smooth functions with compact support on $\mathbb{R}$. Our first duty is then to check whether $\hat{\boldsymbol{H}}$ is essentially self-adjoint on a subspace of $\mathcal{H}$ in order to establish a well-defined quantum theory. For this purpose, a theorem which goes back to Kato [56] is helpful. It states that if the potential energy contribution $V(q,x)$ in $H(q,P,x,y)$ is a measurable, locally bounded function, $V(q,x)\in L^\infty_{\mathrm{loc}}(\mathbb{R}^2)$, and if it is positive $V\geq 0$, then $\hat{\boldsymbol{H}}$, defined as an operator on $C^\infty_{\mathrm{c}}(\mathbb{R}^2)\cong C^\infty_{\mathrm{c}}(\mathbb{R})\otimes C^\infty_{\mathrm{c}}(\mathbb{R})$, is essentially self-adjoint. For our model, the potential energy function V is given by

$$V(q,x) = \frac{1}{2}m\omega_0^2\left(1+\frac{q^2}{L^2}\right)^2\cdot x^2 \tag{13}$$

[cf. Eq. (7)]. V is measurable, locally bounded, and positive. Consequently, $\hat{\boldsymbol{H}}$ is essentially self-adjoint on $C^\infty_{\mathrm{c}}(\mathbb{R}^2)$ and hence generates the time evolution of the quantum states in $\mathcal{H}$. To further analyze the time evolution of the quantum states, it is necessary to resort to a suitable approximation method, for example SAPT, and we therefore alter the representation of the heavy, anharmonic quantum theory. We check the conditions that have to be met for SAPT and adapt the representation accordingly.

B. Checking of the conditions and preparations

We start by checking the conditions (C1)–(C4) for SAPT step by step (cf. Sec. II B). Regarding condition (C1), we note that the tensor product Hilbert space $\mathcal{H} = L^2_{\mathrm{s}}(\mathbb{R})\otimes L^2_{\mathrm{f}}(\mathbb{R})$ of the oscillator model [Eq. (11)] trivially satisfies (C1) because $L^2_{\mathrm{f}}(\mathbb{R})$ is a separable Hilbert space, and hence $\mathcal{H}$ has the required form of a tensor product. Note that as $\mathcal{H}_{\mathrm{f}}$ is separable, it is possible to construct a unique isomorphism between the spaces $L^2(\mathbb{R})\otimes\mathcal{H}_{\mathrm{f}}$ and $L^2(\mathbb{R},\mathcal{H}_{\mathrm{f}})$ [[57], Theorem II.10 on p. 52]. We shortly mention that the $L^2(\mathbb{R},\mathcal{H}_{\mathrm{f}})$ representation of some state $\Psi\in\mathcal{H}$ gives rise to a Hilbert bundle picture: Therefore, consider $\mathcal{M}=\mathbb{R}$ as the base manifold of the Hilbert bundle $H\to\mathcal{M}$ for which every fiber is a Hilbert space $\mathcal{H}_{\mathrm{f}}$. A state $\Psi\in L^2(\mathbb{R},\mathcal{H}_{\mathrm{f}})$ has the form of a section $\Psi: q\mapsto(q,\Psi(q))\in H$ with $\Psi(q)\in\mathcal{H}_{\mathrm{f}}$.

Regarding requirement (C2) which imposes conditions on the Hamilton operator, we start by representing the Hamilton operator as a symbol function $\boldsymbol{H}(q,p)$. Considering a phase space quantization scheme for the heavy oscillator results in the phase space function

$$\boldsymbol{H}(q,p) = \frac{p^2}{2m}\mathbf{1}_{\mathrm{f}} + \frac{\boldsymbol{y}^2}{2m} + \frac{1}{2}m\omega(q)^2\boldsymbol{x}^2, \tag{14}$$

which yields an unbounded operator on $L^2_{\mathrm{f}}(\mathbb{R})$ for every $(q,p)\in\mathbb{R}^2$. Following the space adiabatic perturbation scheme by Panati *et al.* [23], $\boldsymbol{H}(q,p)$ must belong to one of the symbol classes S^m_ρ and therefore should have values in the space of *bounded* operators $\mathcal{B}(L^2_{\mathrm{f}}(\mathbb{R}))$. It is clear that $\boldsymbol{H}$ cannot satisfy this condition as the energy spectrum of the harmonic quantum oscillator is undoubtedly bounded from below but certainly not from above. By using an unbounded operator, we must therefore abstain from the results on the convergence of the perturbative series as proven in [23]. Another possibility, advocated as well in [23] and outlined in Appendix A for our example is to define an auxiliary Hamiltonian that eases these tensions. Since our Hamilton operator is, however, *unbounded*, the resulting auxiliary Hamiltonian is physically different from the original Hamiltonian.

C. Application of space adiabatic perturbation theory

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

We construct a function $\boldsymbol{\pi}_{(1)}(q)$ with values in the bounded operators on $L^2_{\mathrm{f}}(\mathbb{R})$ according to the conditions (S1) in Sec. II C, and with the aim to construct a symbol whose Weyl quantization commutes up to errors of order ε^2 with $\hat{\boldsymbol{H}}$. The construction of the symbol $\boldsymbol{\pi}_{(1)}$ proceeds iteratively using the ansatz of a formal series representation,

$$\boldsymbol{\pi}_{(1)} = \boldsymbol{\pi}_0 + \varepsilon\boldsymbol{\pi}_1. \tag{15}$$

In the first step, the scheme requires one to provide a zeroth order symbol $\boldsymbol{\pi}_0(q)$ as initial data. This must be a projection symbol onto one of the q-dependent eigenspaces of $\boldsymbol{H}(q,p)$ (see Sec. II C). We recall that $\boldsymbol{H}(q,p)$ has the harmonic oscillator eigenfunctions $\xi_n(q)$ as eigensolutions, with q-dependent frequency $\omega(q)$ and constant mass m. The corresponding eigenenergies consist of a generic kinetic energy contribution and the n-dependent oscillator part, i.e., $E_n(q,p) = p^2/(2m) + \omega(q)(n+1/2)$. The zeroth order projection $\boldsymbol{\pi}_0$ is given by one of the eigenprojections $\boldsymbol{\pi}_{0,n}(q) = \xi_n(q)\langle\xi_n(q),\cdot\rangle_{\mathrm{f}}$. In particular, we select one quantum number $n=\nu$ and define the zeroth order symbol to be $\boldsymbol{\pi}_0 \coloneqq \boldsymbol{\pi}_{0,\nu}$. Note that this projector exists for every $(q,p)\in\Gamma_{\mathrm{s}}$ due to the global energy gap. Because of the continuity of the map $(q,p)\mapsto \boldsymbol{H}(q,p)$, the map $(q,p)\mapsto\boldsymbol{\pi}_0(q,p)$ is also continuous. The construction scheme makes use of the star product, here only up to its first order in ε which is given for two symbol functions $\boldsymbol{f}(q,p)$ and $\boldsymbol{g}(q,p)$ by

$$(\boldsymbol{f}\star_\varepsilon\boldsymbol{g})(q,p) = (\boldsymbol{f}\cdot\boldsymbol{g})(q,p) + \frac{i\varepsilon}{2}((\partial_q\boldsymbol{f})\cdot(\partial_p\boldsymbol{g}) - (\partial_p\boldsymbol{f})\cdot(\partial_q\boldsymbol{g}))(q,p) + \mathcal{O}(\varepsilon^2). \tag{16}$$

To shorten the equations, it is reasonable to use the Poisson bracket notation $\{\boldsymbol{f},\boldsymbol{g}\}_{\mathrm{s}} \coloneqq (\partial_q\boldsymbol{f})\cdot(\partial_p\boldsymbol{g}) - (\partial_p\boldsymbol{f})\cdot(\partial_q\boldsymbol{g})$. We follow the steps in Sec. II C and begin by the projector condition (S1–1).

Condition (S1–1) $\boldsymbol{\pi}\star_\varepsilon\boldsymbol{\pi}=\boldsymbol{\pi}$.—The expansion of the first condition (S1–1) in ε yields up to first order with the series expansion of $\boldsymbol{\pi}_{(1)}$ and the star product

$$\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_0 + \varepsilon\left(\frac{i}{2}\{\boldsymbol{\pi}_0,\boldsymbol{\pi}_0\}_{\mathrm{s}} + \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1 + \boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0\right) = \boldsymbol{\pi}_0 + \varepsilon\boldsymbol{\pi}_1 + \mathcal{O}_0(\varepsilon^2). \tag{17}$$

We compare the terms of the same order in ε on both sides of the equation. Regarding the zeroth order, this yields $\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_0=\boldsymbol{\pi}_0$, which holds true by construction. The terms of first order in ε serve to determine $\boldsymbol{\pi}_1$. Since $\boldsymbol{\pi}_0$ does not depend on p, the derivatives $\partial_p\boldsymbol{\pi}_0$ and hence the Poisson bracket vanish. The remaining terms are then $\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1 + \boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0 = \boldsymbol{\pi}_1$. This implies that the diagonal part of the first order symbol $\boldsymbol{\pi}_1$ which is defined as $\boldsymbol{\pi}_1^{\mathrm{D}} \coloneqq \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0 + (\mathbf{1}_{\mathrm{f}}-\boldsymbol{\pi}_0)\cdot\boldsymbol{\pi}_1\cdot(\mathbf{1}_{\mathrm{f}}-\boldsymbol{\pi}_0)$ vanishes. For determining the remaining off-diagonal part $\boldsymbol{\pi}_1^{\mathrm{OD}} \coloneqq \boldsymbol{\pi}_1 - \boldsymbol{\pi}_1^{\mathrm{D}}$, it is necessary to consider the condition (S1–3). Regarding the possible construction of the higher order term $\boldsymbol{\pi}_2$, we note that only $\boldsymbol{\pi}_1$ is helpful for computing the effective Hamiltonian $\boldsymbol{h}_{\mathrm{eff},(2)}$.

Condition (S1–3) $\boldsymbol{H}\star_\varepsilon\boldsymbol{\pi} - \boldsymbol{\pi}\star_\varepsilon\boldsymbol{H}=0$.—The expansion of (S1–3) up to first order in ε yields

$$[\boldsymbol{H},\boldsymbol{\pi}_0]_{\mathrm{f}} + \varepsilon\left(\frac{i}{2}\{\boldsymbol{H},\boldsymbol{\pi}_0\}_{\mathrm{s}} - \frac{i}{2}\{\boldsymbol{\pi}_0,\boldsymbol{H}\}_{\mathrm{s}} + \boldsymbol{H}\cdot\boldsymbol{\pi}_1 - \boldsymbol{\pi}_1\cdot\boldsymbol{H}\right) = \mathcal{O}_0(\varepsilon^2). \tag{18}$$

Again, the zeroth order contribution is trivially satisfied, $[\boldsymbol{H},\boldsymbol{\pi}_0]_{\mathrm{f}}=0$, as the symbol $\boldsymbol{\pi}_0$ is an orthogonal projection operator on the eigensolutions of $\boldsymbol{H}$. The strategy to extract the off-diagonal part of $\boldsymbol{\pi}_1$ is the following: In Eq. (18), we take the first order contributions, and we multiply them by $\boldsymbol{\pi}_0$ from the left and by its orthogonal complement $\boldsymbol{\pi}_0^{\perp} \coloneqq (\mathbf{1}_{\mathrm{f}}-\boldsymbol{\pi}_0)$ from the right. Since $\boldsymbol{\pi}_0$ is the projection on one single eigenspace with eigenenergy E_ν, this factor can be drawn from the left to the right, i.e., $\boldsymbol{\pi}_0\cdot\boldsymbol{H}\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0^{\perp} = \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0^{\perp}E_\nu$. Furthermore, by defining the lower off-diagonal part as $\boldsymbol{\pi}_1^{\mathrm{OD},1} \coloneqq \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0^{\perp}$, we can write for the last two terms $\boldsymbol{\pi}_1^{\mathrm{OD},1}(E_\nu - \boldsymbol{H}^{\perp})$, where $\boldsymbol{H}^{\perp}$ denotes the projection of $\boldsymbol{H}$ on $(\mathbf{1}_{\mathrm{f}}-\boldsymbol{\pi}_0)$. We repeat the procedure for determining $\boldsymbol{\pi}_1^{\mathrm{OD},2} \coloneqq \boldsymbol{\pi}_0^{\perp}\cdot\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0$. In both cases, multiplying $(E_\nu-\boldsymbol{H}^{\perp})^{-1}$ from the right and from the left, respectively, and knowing that the diagonal part of $\boldsymbol{\pi}_1$ vanishes, yields for $\boldsymbol{\pi}_1 = \boldsymbol{\pi}_1^{\mathrm{OD},1} + \boldsymbol{\pi}_1^{\mathrm{OD},2}$

$$\boldsymbol{\pi}_1 = -\frac{i}{2}(\boldsymbol{\pi}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{H}+E_\nu\mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}}\cdot(\boldsymbol{H}^{\perp}-E_\nu\mathbf{1}_{\mathrm{f}})^{-1}\cdot\boldsymbol{\pi}_0^{\perp} + (\boldsymbol{H}^{\perp}-E_\nu\mathbf{1}_{\mathrm{f}})^{-1}\cdot\boldsymbol{\pi}_0^{\perp}\cdot\{\boldsymbol{H}+E_\nu\mathbf{1}_{\mathrm{f}},\boldsymbol{\pi}_0\}_{\mathrm{s}}\cdot\boldsymbol{\pi}_0). \tag{19}$$

For a concrete evaluation of $\boldsymbol{\pi}_1$, it is necessary to know the derivatives of the eigenfunctions $\xi_n(q)$ with respect to q. We use that all excited states $\xi_n(q)$ relate to the vacuum state $\xi_0(q)$ by n-times application of the creation operator $\boldsymbol{a}(q)^*$, namely

$$\xi_n(q) = \frac{(\boldsymbol{a}(q)^*)^n}{\sqrt{n!}}\xi_0(q), \qquad \text{with}\quad \boldsymbol{a}(q)^* = \sqrt{\frac{m\omega(q)}{2}}\left(\boldsymbol{x} - \frac{i}{m\omega(q)}\boldsymbol{y}\right), \tag{20}$$

and where $\boldsymbol{a}(q)^*$ and its adjoint $\boldsymbol{a}(\mathrm{q})$ satisfy the standard commutation relation $[\boldsymbol{a}(\mathrm{q}),\boldsymbol{a}(q)^*]_{\mathrm{f}}=\mathbf{1}_{\mathrm{f}}$. It is straightforward to compute the q-derivative of $\xi_0(q)$ by employing its position representation and keeping track of the q-dependence of the frequency, ω. The explicit q-dependence of $\boldsymbol{a}(q)^*$ is given in (20). The introduction of the function $f(q) \coloneqq -(\partial_q\omega)/(4\omega)$ simplifies the result,

$$\partial_q\xi_0(q) = \sqrt{2}f(q)\xi_2(q), \quad \partial_q\boldsymbol{a}(q)^* = -2f(q)\boldsymbol{a}(\mathrm{q}). \tag{21}$$

The derivative of an excited state $\xi_n(q)$ results from Eqs. (20) and (21), namely

$$\partial_q\xi_n(q) = -\sqrt{n(n-1)}f(q)\xi_{n-2}(q) + \sqrt{(n+1)(n+2)}f(q)\xi_{n+2}(q). \tag{22}$$

We recall that the states $\xi_n(q,x)$ are vectors in $L^2(\mathbb{R}, L^2_{\mathrm{f}}(\mathbb{R}))$, and hence can be seen as sections $\xi_n : q \to (q, \xi_n(q,x))$ of a global Hilbert bundle with $\xi_n(q,x) \in \mathcal{H}_{\mathrm{f}}$. The partial derivative corresponds therefore to a covariant derivative on the space of Hilbert bundle sections $\Gamma(\mathcal{H}_{\mathrm{f}})$, namely $\boldsymbol{\mathcal{A}}(q) : \Gamma(\mathcal{H}_{\mathrm{f}}) \to \Gamma(\mathcal{H}_{\mathrm{f}})$. In order to simplify the equations, we use an index notation with the ξ_n's as basis vectors in $\mathcal{H}_{\mathrm{f}}$. Equation (22) provides the entries of $\boldsymbol{\mathcal{A}}(q)$,

$$\mathcal{A}(q)^k_n = -\sqrt{n(n-1)} f(q) \delta^{k+2}_n + \sqrt{(n+1)(n+2)} f(q) \delta^{k-2}_n. \tag{23}$$

The derivative of the projector $\boldsymbol{\pi}_0(q)$ with respect to q results from the derivation of the states [Eq. (22)] and by using the functional representation of the projector due to Riesz. Besides, we employ the respective elements $\mathcal{A}$ of $\boldsymbol{\mathcal{A}}$,

$$\partial_q \boldsymbol{\pi}_0 = \mathcal{A}(q)^{\nu-2}_{\nu} (\xi_\nu \langle \xi_{\nu-2}, \cdot \rangle_{\mathrm{f}} + \xi_{\nu-2} \langle \xi_\nu, \cdot \rangle_{\mathrm{f}}) + \mathcal{A}(q)^{\nu+2}_{\nu} (\xi_\nu \langle \xi_{\nu+2}, \cdot \rangle_{\mathrm{f}} + \xi_{\nu+2} \langle \xi_\nu, \cdot \rangle_{\mathrm{f}}). \tag{24}$$

It is then straightforward to evaluate the symbol $\boldsymbol{\pi}_1$ by using that $\boldsymbol{\pi}_0$ does not depend on p, but $\boldsymbol{H}$ and E_ν do. In particular, the operator $\partial_p(\boldsymbol{H} + E_\nu \mathbf{1}_{\mathrm{f}})$ is simply $(2p/m) \cdot \mathbf{1}_{\mathrm{f}}$. Furthermore, the inverse of $(\boldsymbol{H}^\perp - E_\nu \mathbf{1}_{\mathrm{f}})$ reduces to a factor $(E_{\nu\pm2} - E_\nu)^{-1} = \pm(2\omega)^{-1}$ when projected on $\xi_{\nu\pm2}$, and we get

$$\boldsymbol{\pi}_1 = \frac{ip}{2m\omega} (\mathcal{A}(q)^{\nu-2}_{\nu} (\xi_\nu \langle \xi_{\nu-2}, \cdot \rangle_{\mathrm{f}} - \xi_{\nu-2} \langle \xi_\nu, \cdot \rangle_{\mathrm{f}}) + \mathcal{A}(q)^{\nu+2}_{\nu} (\xi_{\nu+2} \langle \xi_\nu, \cdot \rangle_{\mathrm{f}} - \xi_\nu \langle \xi_{\nu+2}, \cdot \rangle_{\mathrm{f}})). \tag{25}$$

Condition (S1–2) $\boldsymbol{\pi}^* = \boldsymbol{\pi}$.—It is easy to check that $\boldsymbol{\pi}_{(1)}$ satisfies the condition (S1–2) by transposing and complex conjugating $\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}_1$. For closing this section, we emphasize that $\boldsymbol{\pi}_{(1)}(q,p)$ depends on the heavy phase space variables. After quantization this would yield a nontrivial operator with respect to the heavy subsystem and hence does not simplify the task to find (approximate) solutions for the whole problem. The next step of the scheme therefore consists in constructing a 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 $\mathcal{K}_{\mathrm{f}} \subset \mathcal{H}_{\mathrm{f}}$.

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

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

$$\boldsymbol{\pi}_{\mathrm{p}} := \xi_\nu(q_0) \langle \xi_\nu(q_0), \cdot \rangle_{\mathrm{f}} =: \zeta_\nu \langle \zeta_\nu, \cdot \rangle_{\mathrm{f}}. \tag{26}$$

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

$$\boldsymbol{u}_0(q) := \sum_{n\geq 0} \zeta_n \langle \xi_n(q), \cdot \rangle_{\mathrm{f}}, \tag{27}$$

as initial data of the iteration. This will become clearer when we evaluate the conditions (S2–1) to (S2–3). For the following construction, it is useful to split $\boldsymbol{u}_1$ into a Hermitian and an anti-Hermitian part $\boldsymbol{a}_1 = \boldsymbol{a}_1^*$ and $\boldsymbol{b}_1 = -\boldsymbol{b}_1^*$ such that $\boldsymbol{u}_{(1)} := \boldsymbol{u}_0 + \varepsilon(\boldsymbol{a}_1 + \boldsymbol{b}_1) \cdot \boldsymbol{u}_0$.

Conditions (S2–1) and (S2–2) $\boldsymbol{u} \star_\varepsilon \boldsymbol{u}^* = \mathbf{1}_{\mathrm{f}} = \boldsymbol{u}^* \star_\varepsilon \boldsymbol{u}$.—The given condition of unitarity (S2–1) for $\boldsymbol{u}_1$ evaluates in terms of $\boldsymbol{a}_1$ to the equation

$$\boldsymbol{u}_0 \cdot \boldsymbol{u}_0^* - \mathbf{1}_{\mathrm{f}} + \varepsilon \left(\frac{i}{2} \{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_{\mathrm{s}} + 2\boldsymbol{a}_1 \right) = \mathcal{O}_0(\varepsilon^2), \tag{28}$$

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 (27). Regarding the condition at first order in ε that arises from (28), it is clear that the Poisson bracket $\{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_{\mathrm{s}}$ vanishes since $\boldsymbol{u}_0$ does not depend on p. It therefore follows directly that $\boldsymbol{a}_1 = 0$. The anti-Hermitian part $\boldsymbol{b}_1$ is determined by condition (S2–3).

Condition (S2–3) $\boldsymbol{u} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{u}^* = \boldsymbol{\pi}_{\mathrm{p}}$.—We keep in mind that any Poisson bracket applied on only the symbols $\boldsymbol{\pi}_0$, $\boldsymbol{u}_0$, and $\boldsymbol{u}_0^*$ vanishes, because the symbols do not depend on p. Then, the condition (S2–3) evaluates to

$$\boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}_0^* - \boldsymbol{\pi}_{\mathrm{p}} + \varepsilon([\boldsymbol{b}_1, \boldsymbol{\pi}_{\mathrm{p}}]_{\mathrm{f}} + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1 \cdot \boldsymbol{u}_0^*) = \mathcal{O}_0(\varepsilon^2). \tag{29}$$

It is straightforward to check that our choices of $\boldsymbol{u}_0$, $\boldsymbol{\pi}_0$, and $\boldsymbol{\pi}_{\mathrm{p}}$ satisfy the condition at zeroth order, namely $\boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}_0^* - \boldsymbol{\pi}_{\mathrm{p}} = 0$. At first order in ε, we use that the equation $\boldsymbol{b}_1 = -[\boldsymbol{\pi}_{\mathrm{p}}, [\boldsymbol{b}_1, \boldsymbol{\pi}_{\mathrm{p}}]_{\mathrm{f}}]_{\mathrm{f}}$ gives a solution for $\boldsymbol{b}_1$ which provides the following result for $\boldsymbol{u}_1$:

$$\boldsymbol{u}_1 = [\boldsymbol{\pi}_{\mathrm{p}}, \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1^{\mathrm{OD}} \cdot \boldsymbol{u}_0^*]_{\mathrm{f}} \cdot \boldsymbol{u}_0 \tag{30}$$

$$= \frac{i}{2} \boldsymbol{u}_0 \cdot (\boldsymbol{H}^\perp - E_\nu \mathbf{1}_{\mathrm{f}})^{-1} \cdot \boldsymbol{\pi}_0^\perp \cdot \{\boldsymbol{H} + E_\nu \mathbf{1}_{\mathrm{f}}, \boldsymbol{\pi}_0\}_{\mathrm{s}} \cdot \boldsymbol{\pi}_0 - \frac{i}{2} \boldsymbol{\pi}_{\mathrm{p}} \cdot \boldsymbol{u}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{H} + E_\nu \mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}} \cdot (\boldsymbol{H}^\perp - E_\nu \mathbf{1}_{\mathrm{f}})^{-1} \cdot \boldsymbol{\pi}_0^\perp. \tag{31}$$

The concrete evaluation of $\boldsymbol{u}_1$ in terms of the connections and the eigensolutions ξ_n is given by

$$\boldsymbol{u}_1 = \frac{ip}{2m\omega}(\mathcal{A}(q)_\nu^{\nu-2}(\zeta_\nu\langle\xi_{\nu-2},\cdot\rangle_{\mathrm{f}} + \zeta_{\nu-2}\langle\xi_\nu,\cdot\rangle_{\mathrm{f}}) - \mathcal{A}(q)_\nu^{\nu+2}(\zeta_{\nu+2}\langle\xi_\nu,\cdot\rangle_{\mathrm{f}} + \zeta_\nu\langle\xi_{\nu+2},\cdot\rangle_{\mathrm{f}})). \tag{32}$$

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

The last step of the perturbation scheme consists in pulling the dynamics of the chosen subspace associated with $\boldsymbol{\pi}$ to the ε-independent subspace $\hat{\mathbf{\Pi}}_{\mathrm{p}}\mathcal{H}$. This essentially means that by applying the unitary operator $\hat{\boldsymbol{U}} = \hat{\boldsymbol{u}} + \mathcal{O}_0(\varepsilon^\infty)$ on the Hamiltonian $\hat{\boldsymbol{H}}$, the action of the latter on elements in $\hat{\mathbf{\Pi}}\mathcal{H}$ is rotated to $\hat{\mathbf{\Pi}}_{\mathrm{p}}\mathcal{H}$. The effective Hamiltonian $\hat{\boldsymbol{h}}_{\mathrm{eff}}$ which acts on this subspace is the Weyl quantization of the symbol $\boldsymbol{h}_{\mathrm{eff}}$ which is determined by the condition (S3) in Sec. II C, namely $\boldsymbol{h}_{\mathrm{eff}} = \boldsymbol{u}\star_\varepsilon\boldsymbol{H}\star_\varepsilon\boldsymbol{u}^*$. Again, we assume an ansatz of a formal power series in ε for the effective Hamiltonian, i.e., $\boldsymbol{h}_{\mathrm{eff},(2)} = \boldsymbol{h}_{\mathrm{eff},0} + \varepsilon\boldsymbol{h}_{\mathrm{eff},1} + \varepsilon^2\boldsymbol{h}_{\mathrm{eff},2}$ here up to second order in ε. In the following, we restrict our attention directly to the subspace associated with $\boldsymbol{\pi}_{\mathrm{p}}$ and will project on it. At zeroth order, the condition (S3) gives

$$\boldsymbol{h}_{\mathrm{eff},0,\mathrm{p}} \coloneqq \boldsymbol{\pi}_{\mathrm{p}}\cdot\boldsymbol{u}_0\cdot\boldsymbol{H}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}} = \left(\frac{p^2}{2m} + \omega(q)\left(\nu+\frac{1}{2}\right)\right)\boldsymbol{\pi}_{\mathrm{p}}. \tag{33}$$

For the first and second order contributions in (S3), it is useful to star multiply the condition by $\boldsymbol{u}$ from the right. Thus, the double star product does not have to be carried out. For determining the first order contribution of $\boldsymbol{h}_{\mathrm{eff},1}$, this yields

$$\boldsymbol{u}\star_\varepsilon\boldsymbol{H} - \boldsymbol{h}_{\mathrm{eff},0}\star_\varepsilon\boldsymbol{u} = \varepsilon\boldsymbol{h}_{\mathrm{eff},1}\star_\varepsilon\boldsymbol{u} = \varepsilon\boldsymbol{h}_{\mathrm{eff},1}\cdot\boldsymbol{u}_0 + \mathcal{O}(\varepsilon^2), \tag{34}$$

and by reorganizing the equation

$$\boldsymbol{h}_{\mathrm{eff},1} = \left(\boldsymbol{u}_1\cdot\boldsymbol{H} - \boldsymbol{h}_{\mathrm{eff},0}\cdot\boldsymbol{u}_1 + \frac{i}{2}\{\boldsymbol{u}_0,\boldsymbol{H}\}_{\mathrm{s}} - \frac{i}{2}\{\boldsymbol{h}_{\mathrm{eff},0},\boldsymbol{u}_0\}_{\mathrm{s}}\right)\cdot\boldsymbol{u}_0^*. \tag{35}$$

Knowing that $\boldsymbol{u}_1$ has no diagonal contributions and that $\boldsymbol{u}_0$ does not depend on p, this condition implies that $\boldsymbol{h}_{\mathrm{eff},1}$ has no diagonal contributions. Hence, the restriction to the chosen subspace with quantum number ν vanishes,

$$\boldsymbol{h}_{\mathrm{eff},1,\mathrm{p}} = \frac{i}{2}\boldsymbol{\pi}_{\mathrm{p}}\cdot\{\boldsymbol{u}_0,\boldsymbol{H}+E_\nu\mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}} = 0. \tag{36}$$

The same strategy applies for deriving $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}$. As in Eq. (34), we circumvent the twofold star product by writing

$$\boldsymbol{u}\star_\varepsilon\boldsymbol{H} - (\boldsymbol{h}_{\mathrm{eff},0} + \varepsilon\boldsymbol{h}_{\mathrm{eff},1})\star_\varepsilon\boldsymbol{u} = \varepsilon^2\boldsymbol{h}_{\mathrm{eff},2}\star_\varepsilon\boldsymbol{u} = \varepsilon^2\boldsymbol{h}_{\mathrm{eff},2}\cdot\boldsymbol{u}_0 + \mathcal{O}(\varepsilon^3). \tag{37}$$

The evaluation of the star products on the right-hand side of this equation and multiplication by $\boldsymbol{u}_0^*$ from the right yields

$$\boldsymbol{h}_{\mathrm{eff},2} = ((\boldsymbol{u}_0\star_\varepsilon\boldsymbol{H})_2 + (\boldsymbol{u}_1\star_\varepsilon\boldsymbol{H})_1 + \boldsymbol{u}_2\cdot\boldsymbol{H} - (\boldsymbol{h}_{\mathrm{eff},0}\star_\varepsilon\boldsymbol{u}_0)_2 - (\boldsymbol{h}_{\mathrm{eff},1}\star_\varepsilon\boldsymbol{u}_0)_1 - (\boldsymbol{h}_{\mathrm{eff},0}\star_\varepsilon\boldsymbol{u}_1)_1 - \boldsymbol{h}_{\mathrm{eff},1}\cdot\boldsymbol{u}_1 - \boldsymbol{h}_{\mathrm{eff},0}\cdot\boldsymbol{u}_2)\cdot\boldsymbol{u}_0^*. \tag{38}$$

Several of these contributions vanish when restricting to one single energy band ν by multiplying with $\boldsymbol{\pi}_{\mathrm{p}}$ from the left and the right. First, we have that $\boldsymbol{H}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}} = E_\nu\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}}$ as well as $\boldsymbol{\pi}_{\mathrm{p}}\cdot\boldsymbol{h}_{\mathrm{eff},0} = E_\nu\cdot\boldsymbol{\pi}_{\mathrm{p}}$ such that the third and the last terms containing $\boldsymbol{u}_2$ cancel. As a consequence, the second order contributions to $\boldsymbol{u}$ and $\boldsymbol{\pi}$ do not enter the formula for $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}$. Moreover, the first and the fourth terms in (38) cancel which is due to the fact that the eigenstates $\xi_n(q)$ do not depend on the momentum p. For a detailed proof of this, we refer to Appendix A.3 of the fourth paper of this series [32], more precisely to Eqs. (159) ff.

By evaluating the remaining star products in Eq. (38), we eventually obtain

$$\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}} = \frac{i}{2}\boldsymbol{\pi}_{\mathrm{p}}\cdot\{\boldsymbol{u}_1,\boldsymbol{H}+E_\nu\mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}} - \boldsymbol{\pi}_{\mathrm{p}}\cdot\boldsymbol{h}_{\mathrm{eff},1}\cdot\boldsymbol{u}_1\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}} - \frac{i}{2}\boldsymbol{\pi}_{\mathrm{p}}\cdot\{\boldsymbol{h}_{\mathrm{eff},1},\boldsymbol{u}_0\}_{\mathrm{s}}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\mathrm{p}}. \tag{39}$$

The second order contribution $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}}$ displays the effects of nonadiabaticity. The evaluation of the symbol in (39) yields

$$\boldsymbol{h}_{\mathrm{eff},2,\mathrm{p}} = \frac{L^2}{2m\omega_0}\left(-\frac{p^2q^2}{m(L^2+q^2)^3}\left(\nu+\frac{1}{2}\right) + \frac{q^2}{(L^2+q^2)^2}\frac{\omega_0}{2L^2}(\nu^2+\nu+1)\right)\boldsymbol{\pi}_{\mathrm{p}}. \tag{40}$$

We see that this second order contribution not only gives an additional potential term which only depends on q as a backreaction from the light, harmonic oscillator onto the heavy oscillator. It also yields a kinetic term which depends on the momentum p.

D. Approximate solutions to the effective Hamiltonian

We start with the evaluation of the zeroth order symbol of Eq. (33). It is easy to evaluate the action of its quantization on some generic tensor product wave function in $\mathcal{H} = \mathcal{H}_{\mathrm{s}}\otimes\mathcal{H}_{\mathrm{f}}$: The operator associated with the fast subsystem $\boldsymbol{\pi}_{\mathrm{p}}$ has the eigenfunction ζ_ν, which is the same for every $(q,p)\in\Gamma_{\mathrm{s}}$. Thus, one can simply examine the action of the (q,p)-dependent energy function on

elements of $\mathcal{H}_s$. The Schrödinger equation for some generic wave function $\Psi \in \mathcal{H}_s$, derived from the Hamilton symbol, Eq. (33), is given by

$$\left(-\frac{\partial_q^2}{2M}+\frac{1}{2}M\Omega_\nu^2 q^2\right)\psi^0_{d,\nu}(q)=\tilde{E}_{d,\nu}\psi^0_{d,\nu}(q), \quad (41)$$

where we defined

$$\Omega_\nu=\sqrt{\frac{2\omega_0}{ML^2}\left(\nu+\frac{1}{2}\right)}, \quad \tilde{E}_{d,\nu}=E_{d,\nu}-\omega_0\left(\nu+\frac{1}{2}\right), \quad (42)$$

and $E_{d,\nu}$ is the energy of the whole system. This is the Schrödinger equation of a harmonic oscillator with mass parameter M and frequency Ω_ν. The eigenfunctions $\psi^0_{d,\nu}(q)$ are associated with discrete eigenenergies which are labeled not only by the former quantum number ν of the light subsystem but also by the heavy quantum number d. The superscript "0" indicates that these are the solutions of the *zeroth* order effective Hamiltonian. The respective eigenenergies are given by

$$E_{d,\nu}=\omega_0\left(\nu+\frac{1}{2}\right)+\sqrt{\frac{2\omega_0}{ML^2}\left(\nu+\frac{1}{2}\right)}\cdot\left(d+\frac{1}{2}\right). \quad (43)$$

We emphasize that this result corresponds to the Born-Oppenheimer approximation, i.e., the adiabatic limit of the perturbation theory. In this simplified scheme, the heavy degrees of freedom encounter an external potential given by a single energy level of the light degrees of freedom. This limit is also denoted as the "adiabatic decoupling" because the light degrees of freedom are constrained to stay within one energy band.

The contribution to the effective Hamilton operator of second order, $\hat{\boldsymbol{h}}_{\mathrm{eff},2,\mathrm{p}}$ is the Weyl quantization of the symbol function in Eq. (40). As this operator represents a perturbation of the zeroth order Hamiltonian $\hat{\boldsymbol{h}}_{\mathrm{eff},0,\mathrm{p}}$, standard quantum mechanical perturbation theory applies and provides corrections to the spectrum $\{E_{d,\nu}\}_{d\in\mathbb{N}}$. Namely, the shift of the energy due to $\hat{\boldsymbol{h}}_{\mathrm{eff},2,\mathrm{p}}$ is given as the expectation value in the zeroth order states, i.e., $\Delta E_{d,\nu} \coloneqq \langle \psi^0_{d,\nu}, \hat{\boldsymbol{h}}_{\mathrm{eff},2,\mathrm{p}}\psi^0_{d,\nu}\rangle_s$. Knowing both ingredients, the zeroth order states and the form of the perturbation effective Hamiltonian, it is straightforward to compute $\Delta E_{d,\nu}$ for any d and ν in $\mathbb{N}$. We present the derivations and the explicit formulas in Appendix B and content ourselves with providing the expression for $\Delta E_{0,\nu}$ for illustration here. Therefore, we define a dimensionless parameter $\ell_\nu \coloneqq \sqrt{M\Omega_\nu}L$, and we obtain

$$\begin{aligned}\Delta E_{0,\nu}=&-\frac{\Omega_\nu}{4}(\nu^2+\nu+1)+\frac{\Omega_\nu^2}{16\omega_0}\left(\nu+\frac{1}{2}\right)(2+7\ell_\nu^2+2\ell_\nu^4)\\&+\mathrm{Erf}(\ell_\nu)\frac{\sqrt{\pi}e^{\ell_\nu^2}}{8\ell_\nu}\left(\frac{\Omega_\nu^2(\nu+\frac{1}{2})}{4\omega_0}(11\ell_\nu^2-2\right.\\&\left.+20\ell_\nu^4+4\ell_\nu^6)-\Omega_\nu(\nu^2+\nu+1)(1+2\ell_\nu^2)\right), \quad (44)\end{aligned}$$

where $\mathrm{Erf}(\ell_\nu)=\mathrm{erf}(\ell_\nu)-1$, with "erf" being the standard error function.

IV. COSMOLOGICAL MODEL

A. Presentation of the system and preparations

This second showcase example for applying SAPT analyzes a simple cosmological scenario: We consider Einstein general relativity on a globally hyperbolic spacetime manifold $\mathcal{M}$, reduced to spatial homogeneity and isotropy, including a cosmological constant $\Lambda \in \mathbb{R}^+$ and coupled to a spatially homogeneous, isotropic, and real-valued Klein-Gordon field ϕ with mass $m \in \mathbb{R}^+$. The background space manifold is the compact three-torus $\mathbb{T}^3$ with coordinate side length l in all three directions and flat spatial slices, i.e., $k=0$ in the standard notation. The spacetime manifold is thus modeled by $\mathcal{M}=\mathbb{R}\times\mathbb{T}^3$. We choose coordinates such that the time parameter t labels the homogeneous and isotropic spatial slices. The metric tensor g of general relativity has the scale factor $a \in \mathbb{R}^+$ as its only remaining dynamical degree of freedom. The scalar field reduces to a homogeneous and isotropic variable, $\phi \in \mathbb{R}$. Both a and ϕ depend on the time parameter t. The Einstein-Hilbert and the matter field "cosmological" action are given by

$$S[a,\phi]=l^3\int_{\mathbb{R}}\mathrm{d}t\left(-\frac{1}{2\kappa}(6\dot{a}^2a+2\Lambda a^3)+\frac{1}{2\lambda}a^3(\dot{\phi}^2-m^2\phi^2)\right), \quad (45)$$

where the integration over the torus volume produces a factor l^3. Here, κ and λ are, respectively, the coupling constants of general relativity and the Klein-Gordon system, where $\kappa=8\pi G$ and G is Newton's constant. If both (a,ϕ) are dimensionless, as we assume, then both coupling constants have the same dimension. Our motivation for this choice is that in this way we do not need to introduce additional mass scales into more general than quadratic inflaton potentials. Thus, it is reasonable to define the adiabatic perturbation parameter as the dimensionless ratio,

$$\varepsilon^2 \coloneqq \frac{\kappa}{\lambda}. \quad (46)$$

Note that we can associate mass parameters to the coupling constants, namely $m_\lambda^2 \coloneqq \lambda^{-1}$ and $M_{\mathrm{Pl}}^2 \coloneqq \kappa^{-1}$ where M_{Pl} is the reduced Planck mass. Note that we set $\hbar=1=c$ throughout this section. We assume that $m_\lambda \ll M_{\mathrm{Pl}}$ and thus

$\varepsilon \ll 1$, which is certainly the case if m_λ is in the mass range of a typical Standard Model particle mass. We also point out that λ and the mass of the scalar (inflaton) field m are *independent* parameters.

Note that in the usual considerations of inflation, λ is generically set to one. This is of course a choice and has no consequences for the physical content of the theory. By allowing different values for λ, we simply introduce a (physically irrelevant) parametrization invariance for the scalar field.

It transpires that in the adiabatic language, gravity is the "slow" sector and the Klein-Gordon particle the "fast" one. This may seem counterintuitive when one thinks of the Klein-Gordon field as an inflaton candidate and the inflationary phase when ϕ practically freezes (for small m) while a expands exponentially. However, note that the distinction of slow and fast degrees of freedom uses intrinsically a statistical average over the phase space. For instance, when the system under consideration has a true Hamiltonian bounded from below, one uses the equipartition theorem (see Ref. [24] and references therein). In our case, we do not have a true Hamiltonian but rather a Hamiltonian constraint so that the equipartition theorem does not apply. However, we can use the constraint itself (basically the Friedmann equation) to deduce that for the velocities, $u = \ln(\dot{a})$ and $v = \dot{\phi}$, it holds that $u^2/\kappa \approx v^2/\lambda$ for small Λ/κ in scalar field kinetic energy dominated parts of the phase space. See the companion paper [24] for more details.

The space adiabatic scheme requires a Hamiltonian formulation of the problem. We define the conjugate momenta of a and ϕ as $p_a := \varepsilon \frac{\partial L}{\partial \dot{a}}$ and $\mu := \frac{\partial L}{\partial \dot{\phi}}$ where L is the Lagrange function associated with the action S. The Poisson brackets of the canonical variables evaluate to $\{a, p_a\} = \varepsilon$ and $\{\phi, \mu\} = 1$. This choice for the fundamental Poisson relations assures that we can identify the masses associated with the homogeneous and isotropic degrees of freedom with the mass of the total system of the torus as pointed out in [24]. The Legendre transformation generates the Hamilton constraint,

$$C(a, p_a, \phi, \mu) := -\frac{1}{12}\frac{p_a^2}{a} + \frac{\Lambda}{\lambda\kappa}a^3 + \frac{\mu^2}{2a^3} + \frac{1}{2\lambda^2}m^2 a^3 \phi^2, \quad (47)$$

where for notational reasons, we divided the whole constraint by a constant factor λ. Besides, we set $l^3 = 1$ without loss of generality. For simplifying the analysis by means of space adiabatic perturbation theory in the following, we switch to "triadlike" canonical variables,

$$b := \pm\sqrt{a^3}, \qquad \rho := \frac{2}{3}\frac{p_a}{\sqrt{a}}, \quad (48)$$

which is a double cover of the original phase space. Note that the range of b consists of two branches, a positive and a negative one. We do not restrict to any of them. In order to keep the notation as simple as possible, we introduce the following parameters and functions:

$$m_{\mathrm{G}} := \frac{8}{3}, \quad \omega_{\mathrm{G}}^2 := \frac{3\Lambda}{4\lambda\kappa}, \quad \tilde{m}_{\mathrm{KG}} := b^2, \quad \omega_{\mathrm{KG}}^2 := \frac{m_{\mathrm{KG}}^2}{\lambda^2}. \quad (49)$$

These definitions and the new canonical variables give for the Hamilton constraint

$$C(b, \rho, \phi, \mu) = -\frac{\rho^2}{2m_{\mathrm{G}}} + \frac{1}{2}m_{\mathrm{G}}\omega_{\mathrm{G}}^2 b^2 + \frac{\mu^2}{2\tilde{m}_{\mathrm{KG}}(b)} + \frac{1}{2}\tilde{m}_{\mathrm{KG}}(b)\omega_{\mathrm{KG}}^2\phi^2. \quad (50)$$

We quantize the system and start by considering the scalar field subsystem. The state space is the standard L^2-Hilbert space and will be denoted by $\mathcal{H}_{\mathrm{f}} = L_{\mathrm{f}}^2(\mathbb{R})$. The quantum operators are indicated as bold, and the scalar field operator and its conjugate momentum satisfy the canonical commutation relation $[\boldsymbol{\phi}, \boldsymbol{\mu}]_{\mathrm{f}} = i\mathbf{1}_{\mathrm{f}}$. Similarly, the state space of the geometrical subsystem will be denoted by $\mathcal{H}_{\mathrm{s}} = L_{\mathrm{s}}^2(\mathbb{R})$. The quantum operators wear hats and the canonical commutation relation for the geometrical variable and its conjugate momentum are $[\hat{b}, \hat{\rho}]_{\mathrm{s}} = i\varepsilon\hat{\mathbf{1}}_{\mathrm{s}}$. The quantum theory of the coupled system has the tensor product Hilbert space $\mathcal{H}_{\mathrm{s}} \otimes \mathcal{H}_{\mathrm{f}}$. Note that this is not the representation chosen in loop quantum cosmology (LQC) [58–60] for which one motivation is that inverse powers of a or b can be made well-defined following the technique introduced for loop quantum gravity (LQG) [61,62]. That technique does not work in the presently chosen Schrödinger representation. However, one can still find a dense and invariant domain [63] for the Hamiltonian constraint operator of the full system which is sufficient to perform the spectral analysis. The constraint operator on the tensor product Hilbert space is given by

$$\hat{\boldsymbol{C}} = \left(-\frac{\hat{\rho}^2}{2m_{\mathrm{G}}} + \frac{1}{2}m_{\mathrm{G}}\omega_{\mathrm{G}}^2\hat{b}^2\right) \otimes \mathbf{1}_{\mathrm{f}} + \frac{1}{2\tilde{m}_{\mathrm{KG}}(\hat{b})} \otimes \boldsymbol{\mu}_0^2 + \frac{1}{2}\tilde{m}_{\mathrm{KG}}(\hat{b})\omega_{\mathrm{KG}}^2 \otimes \boldsymbol{\phi}_0^2. \quad (51)$$

This operator is, due to the inverse kinetic energy operator of the geometric sector, not bounded from below. In fact, it is a constraint, and we are mostly interested in the domain of the Hilbert space that is annihilated by the constraint. Exact solutions are obviously not available. In what follows, we perform a systematic step by step SAPT treatment.

B. Checking of the conditions and preparations

We check the conditions (C1)–(C4) from Sec. II B for the cosmological model. Condition (C1) holds without further ado since the cosmological Hilbert space $\mathcal{H}_{\mathrm{s}} \otimes \mathcal{H}_{\mathrm{f}}$ has the required tensor product form. In addition, $\mathcal{H}_{\mathrm{s}}$ is an L^2-space and $\mathcal{H}_{\mathrm{f}}$ is a separable Hilbert space. Following condition

(C2), we represent the quantum constraint (51) as a symbol function $\boldsymbol{C}(b,\rho)$ with values in the linear operators on the Klein-Gordon Hilbert space $\mathcal{H}_{\mathrm{f}}$. Formally, we simply quantize the Klein-Gordon subsystem by means of a standard Weyl quantization procedure and obtain

$$\boldsymbol{C}(b,\rho) = \left(-\frac{\rho^2}{2m_{\mathrm{G}}} + \frac{1}{2}m_{\mathrm{G}}\omega_{\mathrm{G}}^2 b^2\right)\mathbf{1}_{\mathrm{f}} + \frac{\boldsymbol{\phi}^2}{2\tilde{m}_{\mathrm{KG}}(b)} + \frac{1}{2}\tilde{m}_{\mathrm{KG}}(b)\omega_{\mathrm{KG}}^2\boldsymbol{\mu}^2. \tag{52}$$

This symbol function is an unbounded operator on $\mathcal{H}_{\mathrm{f}}$ for every $(b,\rho) \in \mathbb{R}^2$. In particular, the operator corresponds to the Hamiltonian of a quantum harmonic oscillator with constant frequency ω_{KG}, b-dependent mass $\tilde{m}_{\mathrm{KG}}(b)$, and an offset energy. As such, the symbol has an energy spectrum which is unbounded. According to SAPT, the constraint symbol must belong to one of the symbol classes S^m_ρ and should therefore have values in the space of *bounded* operators on $\mathcal{H}_{\mathrm{f}}$. Furthermore, it must be a bounded function with respect to the geometric variable b and grow maximally polynomially with respect to ρ. This is not the case because the constraint contains terms proportional to $\tilde{m}_{\mathrm{KG}}(b) = b^2$ and its inverse.

In fact, we could now apply the same strategy as introduced in the previous section and define a suitable auxiliary Hamilton symbol $\boldsymbol{H}_{\mathrm{aux}}$ to which one finally applies SAPT. This nontrivial task will, however, not be able to account for the properties and dynamics generated by the original Hamilton constraint, as already mentioned. Therefore, we will again abandon the convergence results for bounded operators as presented in [23] and remain with the original Hamilton constraint for our application of SAPT.

C. Application of space aAdiabatic perturbation theory

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

According to the iterative scheme presented in Sec. II C, we construct a function $\boldsymbol{\pi}_{(1)}(b)$ with values in the bounded operators on $L^2_{\mathrm{f}}(\mathbb{R})$. We use the ansatz of a formal power series $\boldsymbol{\pi}_{(1)} = \boldsymbol{\pi}_0 + \varepsilon\boldsymbol{\pi}_1$ and the conditions subsumed in (S1). In the first step, the scheme requires one to provide the zeroth order symbol $\boldsymbol{\pi}_0(b)$ as initial data which must be the projection symbol onto one of the b-dependent eigenspaces of $\boldsymbol{C}(b,\rho)$. As $\boldsymbol{C}(b,\rho)$ is the Hamilton operator of a harmonic oscillator with b-dependent mass $\tilde{m}_{\mathrm{KG}}(b)$, constant frequency ω_{KG}, and an offset energy, $\boldsymbol{\pi}_0(b)$ is simply the eigenprojection onto one of the eigensolutions, $\xi_n(b)$, with

$$\boldsymbol{C}(b,\rho)\xi_n(b) = E_n(b,\rho)\xi_n(b), \tag{53}$$

where we introduced the (b,ρ)-dependent, discrete energy spectrum

$$E_n(b,\rho) = -\frac{\rho^2}{2m_{\mathrm{G}}} + \frac{1}{2}m_{\mathrm{G}}\omega_{\mathrm{G}}^2 b^2 + \omega_{\mathrm{KG}}\left(n+\frac{1}{2}\right). \tag{54}$$

The eigensolutions $\xi_n(b)$ are the harmonic oscillator eigenfunctions with b-dependent mass $\tilde{m}_{\mathrm{KG}}(b)$ and constant frequency ω_{KG}. With these prerequisites, the scheme suggests to select one quantum number $n = \nu$, and to define $\boldsymbol{\pi}_0(b) \coloneqq \xi_\nu(b)\langle\xi_\nu(b),\cdot\rangle_{\mathrm{f}}$. Again, we note that $\boldsymbol{\pi}_0(b)$ is a continuous function with respect to b (cf. Sec. III C 1). Then, following the instructions from Sec. II C and the steps taken in the example of the oscillator model (cf. Sec. III C 1), the projector symbol has the form

$$\boldsymbol{\pi}_1 = -\frac{i}{2}(\boldsymbol{\pi}_0\cdot\{\boldsymbol{\pi}_0,\boldsymbol{C}+E_\nu\mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}}\cdot(\boldsymbol{C}^\perp - E_\nu\mathbf{1}_{\mathrm{f}})^{-1}\cdot\boldsymbol{\pi}_0^\perp + (\boldsymbol{C}^\perp - E_\nu\mathbf{1}_{\mathrm{f}})^{-1}\cdot\boldsymbol{\pi}_0^\perp\cdot\{\boldsymbol{C}+E_\nu\mathbf{1}_{\mathrm{f}},\boldsymbol{\pi}_0\}_{\mathrm{s}}\cdot\boldsymbol{\pi}_0), \tag{55}$$

where $\boldsymbol{C}^\perp = \boldsymbol{C}\cdot(\mathbf{1}_{\mathrm{f}} - \boldsymbol{\pi}_0)$. For the concrete evaluation of $\boldsymbol{\pi}_1$, it is reasonable to resort to a representation in terms of annihilation and creation operators $\boldsymbol{a}(\mathrm{b})$ and $\boldsymbol{a}(b)^*$ of the problem. These satisfy the canonical commutation relations $[\boldsymbol{a}(\mathrm{b}),\boldsymbol{a}(b)^*]_{\mathrm{f}} = \mathbf{1}_{\mathrm{f}}$, and the creation operator is given by

$$\boldsymbol{a}(b)^* = \sqrt{\frac{\tilde{m}_{\mathrm{KG}}(b)\omega_{\mathrm{KG}}}{2}}\left(\boldsymbol{\phi} - \frac{i}{\tilde{m}_{\mathrm{KG}}(b)\omega_{\mathrm{KG}}}\boldsymbol{\mu}\right). \tag{56}$$

Using the b-dependence of the oscillator eigenfunction $\xi_0(b)$ with mass $\tilde{m}_{\mathrm{KG}}(b)$ and of $\boldsymbol{a}(b)^*$, their derivatives are simply

$$\partial_b\xi_0(b) \coloneqq \sqrt{2}f(b)\xi_2(b), \quad \partial_b\boldsymbol{a}(b)^* = -2f(b)\boldsymbol{a}(b), \tag{57}$$

where we have introduced the function $f(b) \coloneqq -(\partial_b\tilde{m}_{\mathrm{KG}})/(4\tilde{m}_{\mathrm{KG}}) = -1/(2b)$. As a consequence, the b-derivative of the excited states have the form

$$\partial_b\xi_n(b) = \mathcal{A}(b)_n^{n-2}\xi_{n-2}(b) + \mathcal{A}(b)_n^{n+2}\xi_{n+2}(b), \tag{58}$$

where we used that any excited state derives from the vacuum state by multiple applications of the creation operator and the same definition for the elements of the covariant derivative $\boldsymbol{\mathcal{A}}$ as for the oscillator model. In analogy, the operator $\partial_b(\boldsymbol{C} - E_\nu\cdot\mathbf{1}_{\mathrm{f}})$ is simply $(-2p/m_{\mathrm{G}})\cdot\mathbf{1}_{\mathrm{f}}$, and the inverse of $(\boldsymbol{C}^\perp - E_\nu)$ reduces to a factor of $\pm(2\omega_{\mathrm{KG}})^{-1}$. As a result, the projector symbol $\boldsymbol{\pi}_1$ has the form

$$\boldsymbol{\pi}_1 = -\frac{i\rho}{2m_{\mathrm{G}}\omega_{\mathrm{KG}}}(\mathcal{A}(b)_\nu^{\nu-2}(\xi_\nu\langle\xi_{\nu-2},\cdot\rangle_{\mathrm{f}} - \xi_{\nu-2}\langle\xi_\nu,\cdot\rangle_{\mathrm{f}}) + \mathcal{A}(b)_\nu^{\nu+2}(\xi_{\nu+2}\langle\xi_\nu,\cdot\rangle_{\mathrm{f}} - \xi_\nu\langle\xi_{\nu+2},\cdot\rangle_{\mathrm{f}})). \tag{59}$$

One can check that $\boldsymbol{\pi}_{(1)}$ satisfies all three conditions subsumed under (S1) up to first order in ε. Again, the next step consists in unitarily mapping the dynamics within the subspace associated with $\boldsymbol{\pi}_1$ to a simpler reference subspace.

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

Analogous to the proceeding in Sec. III C 2, we construct a unitary symbol $\boldsymbol{u}_{(1)}$ which maps the dynamical subspace related to $\boldsymbol{\pi}_{(1)}$ to a suitable reference subspace $\mathcal{K}_{\mathrm{f}} \subset \mathcal{H}_{\mathrm{f}}$. We select one fixed $(b_0, \rho_0) \in \Gamma_{\mathrm{s}}$ and define the reference projection as

$$\boldsymbol{\pi}_{\mathrm{p}} := \xi_\nu(b_0)\langle \xi_\nu(b_0), \cdot\rangle_{\mathrm{f}} =: \zeta_\nu \langle \zeta_\nu, \cdot\rangle_{\mathrm{f}}. \tag{60}$$

The unitary operator in line with the conditions (S2) at zeroth order is given by

$$\boldsymbol{u}_0(b) = \sum_{n\geq 0} \zeta_n \langle \xi_n(b), \cdot\rangle_{\mathrm{f}}. \tag{61}$$

The iterative construction gives in analogy to the results in Sec. III C 2 for $\boldsymbol{u}_1$

$$\begin{aligned}\boldsymbol{u}_1 &= [\boldsymbol{\pi}_{\mathrm{p}}, \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1^{\mathrm{OD}} \cdot \boldsymbol{u}_0^*]_{\mathrm{f}} \cdot \boldsymbol{u}_0 \\ &= \frac{i\rho}{2m_{\mathrm{G}}\omega_{\mathrm{KG}}} (\mathcal{A}(b)_\nu^{\nu-2} (\zeta_\nu \langle \xi_{\nu-2}, \cdot\rangle_{\mathrm{f}} + \zeta_{\nu-2}\langle \xi_\nu, \cdot\rangle_{\mathrm{f}}) \\ &\quad - \mathcal{A}(b)_\nu^{\nu+2} (\zeta_{\nu+2}\langle \xi_\nu, \cdot\rangle_{\mathrm{f}} + \zeta_\nu \langle \xi_{\nu+2}, \cdot\rangle_{\mathrm{f}})).\end{aligned} \tag{62}$$

3. Construction of the effective constraint symbol $h_{\mathbf{eff},(2)}$

The last step of the perturbation scheme consists in computing an effective Hamilton constraint as a formal power series in ε up to second order. In particular, we restrict ourselves to the computation of the effective Hamiltonian within the selected reference space, i.e., $\boldsymbol{C}_{\mathrm{eff},(2),\mathrm{p}}(b,\rho) := \boldsymbol{\pi}_{\mathrm{p}} \cdot \boldsymbol{C}_{\mathrm{eff},(2)}(b,\rho) \cdot \boldsymbol{\pi}_{\mathrm{p}}$. The zeroth order contribution of this symbol is given according to condition (S3) restricted to zeroth order by

$$\boldsymbol{C}_{\mathrm{eff},0,\mathrm{p}}(b,\rho) = \left(-\frac{\rho^2}{2m_{\mathrm{G}}} + \frac{1}{2} m_{\mathrm{G}} \omega_{\mathrm{G}}^2 b^2 + \omega_{\mathrm{KG}}\left(\nu + \frac{1}{2}\right)\right)\boldsymbol{\pi}_{\mathrm{p}}. \tag{63}$$

Thus, the effective constraint symbol for the gravitational degrees of freedom includes the bare gravitational constraint symbol plus an offset energy which stems from Klein-Gordon's particle chosen energy value. This result corresponds to the Born-Oppenheimer approximation. As in the oscillator model, the first order contribution of the effective constraint symbol, $\boldsymbol{C}_{\mathrm{eff},1}(b,\rho)$, contains only off-diagonal terms, such that $\boldsymbol{C}_{\mathrm{eff},1,\mathrm{p}}(b,\rho)$ vanishes,

$$\boldsymbol{C}_{\mathrm{eff},1,\mathrm{p}}(b,\rho) = \frac{i}{2}\boldsymbol{\pi}_{\mathrm{p}} \cdot \{\boldsymbol{u}_0, \boldsymbol{C} + E_\nu \mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\mathrm{p}} = 0. \tag{64}$$

The same reasoning used for the computation of $\boldsymbol{C}_{\mathrm{eff},1,\mathrm{p}}(b,\rho)$ gives for the second order contribution a similar result as for the oscillator model [see Eq. (39)]. The explicit symbol for the cosmological model is thus

$$\begin{aligned}\boldsymbol{C}_{\mathrm{eff},2,\mathrm{p}}(b,\rho) = \frac{1}{2m_{\mathrm{G}}\omega_{\mathrm{KG}}} &\left(-\frac{\rho^2}{\omega_{\mathrm{G}} b^2}\left(\nu + \frac{1}{2}\right)\right. \\ &\left. - \frac{1}{b^2}\frac{\omega_{\mathrm{KG}}}{2}(\nu^2 + \nu + 1)\right)\boldsymbol{\pi}_{\mathrm{p}}.\end{aligned} \tag{65}$$

This proves our statement that besides the trivial Born-Oppenheimer approximation, further backreaction effects arise for the gravitational subsystem. It is now easy to evaluate the action of this symbol on some generic tensor product wave function in $\mathcal{H} = \mathcal{H}_{\mathrm{s}} \otimes \mathcal{H}_{\mathrm{f}}$, since the Klein-Gordon tensor factor does not depend on the gravitational degrees of freedom anymore.

4. Solutions of the effective constraint operator

The final step consists in the Weyl quantization of the effective Hamiltonian symbols constructed above up to second order in the adiabatic parameter which consists of the two contributions (63) and (65) of zeroth and second order, respectively. The zeroth order contribution has no ordering ambiguities and represents essentially an inverted harmonic oscillator with nonvanishing zero point energy. The second order contribution becomes symmetrically Weyl ordered in this step and involves negative powers of b, which thus is more singular than the zeroth order contribution. The spectral problem of the zeroth order contribution is the one of an inverted oscillator, well studied in the literature (see, e.g., Ref. [42] and references therein). The spectrum is of the absolutely continuous type, and the operator is essentially self-adjoint on the space of smooth functions vanishing at infinity. The generalized (i.e., not normalizable) eigenvectors are explicitly known in terms of parabolic cylinder functions. It is possible to choose boundary conditions such that these eigenfunctions vanish at zero where the classical singularity resides. One would now like to proceed as for the oscillator model and treat the second order contribution as a small correction to the second order by means of stationary perturbation theory. Unfortunately, this method is applicable only when the zeroth order has a pure point spectrum. In fact, it is well known that the perturbation theory for absolutely continuous operators is very unstable in the sense that a perturbation by an operator of an arbitrarily small Hilbert-Schmidt norm exists such that their sum has a pure point spectrum [41]. We are not aware of any rigorous work in that direction, and it seems that the spectral problem of the Hamiltonian constraint operator including zeroth and second order contributions must be addressed by independent methods such as using the dense and invariant domain studied in [63]. We leave this problem for future research and just point out once more how nontrivial the inclusion of backreaction effects can become.

V. CONCLUSION AND OUTLOOK

We applied SAPT to two closely related quantum mechanical models: We first studied a quantum mechanical system of a heavy and slow anharmonic oscillator which is coupled to a lighter and fast harmonic oscillator. The coupling has been established via the potential term in the Hamilton operator. The motivation for this model has been of a technical nature and served as a preparation for the second, cosmological model. There, we considered the purely homogeneous sector of quantum cosmology in order to study the influence of backreaction between geometry and matter contributions to the Hamiltonian constraint. This influence can be encoded in terms of a purely gravitational effective Hamiltonian which receives corrections from the backreactions of the matter degrees of freedom that one would not expect in a crude Born-Oppenheimer approximation. These correction terms could play an important role in the details of a possible singularity resolution that was discovered in the LQC approach to quantum cosmology [58–60].

While we have not done so in this paper, one could of course also quantize the slow sector using such loop methods. Therefore, the phase space quantization scheme needs to be revisited as the standard procedure here relies on the Weyl quantization ordering. In particular, the standard phase space $T^*(\mathbb{R})$ would have to be replaced by $T^*(S^1)$ which was already done in [36–38]. We have not done so, because [63] shows that there exists a dense and invariant domain for the Hamiltonian constraint and all its finite order backreaction terms; in particular all matrix elements can be computed in closed form. We will come back to the phenomenological consequences of backreactions for the model discussed in this paper in future publications.

In the two remaining papers of this series, we employ quantum field theory by taking the inhomogeneous degrees of freedom to linear order in cosmological perturbation theory into account [31,32]. We meet additional challenges as was already explained in [24]: In order to secure unitary equivalence of the different Fock spaces for different homogeneous configurations, one must perform additional transformations for the whole canonical system in linear cosmological perturbation theory. Such transformations were constructed in [64,65] and can be applied for our purposes. The implementation of such transformations can lead to tachyonic quantum fields in some parts of the slow (homogeneous) phase space. An example for a (gauge invariant) quantum field with an indefinite mass squared term is the Mukhanov-Sasaki scalar perturbation in cosmology. Hence, the occurrence of such instabilities in our considerations is *not* due to the SAPT scheme itself and is already encountered in standard gauge-invariant cosmological perturbation theory [66]. In [24], we have made several proposals for overcoming the corresponding problems including a phase space restriction induced by an additional partial canonical transformation in the homogeneous sector, and we will apply them in [31,32].

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APPENDIX A: REGULATION OF THE HAMILTON SYMBOL

It is possible to define an auxiliary Hamilton symbol $\boldsymbol{H}_{\mathrm{aux}}(q,p)$ which is not only a bounded operator on $\mathcal{H}_{\mathrm{f}}$ but also a bounded function with respect to the slow phase space variables q and p. Therefore it is helpful to rewrite the Hamilton symbol $\boldsymbol{H}(q,p)$ in its spectral form using that the problem corresponds to a harmonic oscillator with q-dependent frequency $\omega(q)$, mass m, energy offset $E_{\mathrm{off}}(p) \coloneqq \frac{p^2}{2m}$, and eigensolutions $\xi_n(q) \in \mathcal{H}_{\mathrm{f}}$, $n \in \mathbb{N}$ with energy eigenfunctions $E_n(q,p)$,

$$\begin{aligned}\boldsymbol{H}(q,p)\xi_n(q) &= E_n(q,p)\xi_n(q),\\ E_n(q,p) &\coloneqq E_{\mathrm{off}}(p) + \omega(q)\left(n+\frac{1}{2}\right).\end{aligned} \tag{A1}$$

The q-dependent projectors on $\mathcal{H}_{\mathrm{f}}$ are simply given by

$$\boldsymbol{\pi}_n(q) \coloneqq \xi_n(q)\langle \xi_n(q), \cdot\rangle_{\mathrm{f}}, \tag{A2}$$

where $\langle\cdot,\cdot\rangle_{\mathrm{f}}$ denotes the standard scalar product in $\mathcal{H}_{\mathrm{f}}$. As a consequence, the Hamiltonian symbol in its spectral form is given by

$$\boldsymbol{H}(q,p) = \sum_{n\geq 0} E_n(q,p)\boldsymbol{\pi}_n(q). \tag{A3}$$

Following the strategy in [23], let us define a cutoff Hamiltonian symbol $\boldsymbol{H}_N(q,p)$ with values in the bounded operators on $\mathcal{H}_{\mathrm{f}}$,

$$\boldsymbol{H}_N(q,p) \coloneqq \sum_{n=0}^{N} E_n(q,p)\boldsymbol{\pi}_n(q), \tag{A4}$$

whose norm is $E_N(q,p)$. In order to satisfy condition (C4) for a constant gap, it is necessary to define another "auxiliary" Hamiltonian $\boldsymbol{H}_{\mathrm{aux}}(q,p)$. The idea is to replace the function $\boldsymbol{H}_N(q,p)$ by some appropriately bounded

function outside a certain compact region on the slow phase space. Therefore, let us define the interval $\Lambda \coloneqq \{(q,p) : \|\boldsymbol{H}_N(q,p)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} < E_\mathrm{c}\}$, or more precisely, all points $(q,p) \in \mathbb{R}^2$ for which it holds true that $E_N(q,p) < E_\mathrm{c}$. Therefore, we need $E_\mathrm{c} > \omega_0(N+1/2)$. The auxiliary Hamiltonian symbol must then satisfy [[23], p. 176]

(i) $\boldsymbol{H}_\mathrm{aux}(q,p) = \boldsymbol{H}_N(q,p)$ for all $(q,p) \in \Lambda + \mu \coloneqq \{(q,p) : \|\boldsymbol{H}_N(q,p)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} < E_\mathrm{c} + \mu\}$,

(ii) $\|\boldsymbol{H}_\mathrm{aux}(q,p)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} > \|\boldsymbol{H}_N(q',p')\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})}$ for all $(q,p) \notin \Lambda + \mu$ and $(q',p') \in \Lambda + \mu$,

(iii) $\boldsymbol{H}_\mathrm{aux}(q,p)$ satisfies the global gap condition with $\gamma = 0$, i.e., a constant gap.

$\boldsymbol{H}_\mathrm{aux}$ can be obtained by smoothly extending the energy bands $E_n(q,p)$ outside of the region $\Lambda + \mu$ by a set of bounded, smooth functions with appropriate transition conditions, for example,

$$\boldsymbol{H}_\mathrm{aux}(q,p) = \sum_{n=0}^{N} \tilde{E}_n(q,p)\boldsymbol{\pi}_n(q),$$
$$\text{with} \quad \tilde{E}_n(q) = \begin{cases} E_n(q,p) & \text{if } (q,p) \in \Lambda + \mu, \\ b_n(q,p) & \text{if } (q,p) \notin \Lambda + \mu, \end{cases} \tag{A5}$$

where $b_n(q,p) \in C_\mathrm{b}^\infty(\mathbb{R}^2, \mathbb{R})$ is an appropriately bounded function for every $0 \le n \le N$. Besides, they must be pointwise distinct; i.e., they are not allowed to merge into or to cross with one another. This is important for the gap condition (C3). In fact, with these requirements, $\boldsymbol{H}_\mathrm{aux}(q,p)$ satisfies all conditions for SAPT.

Finally it is possible to show that the dynamics of $\hat{\boldsymbol{H}}_N$ and $\hat{\boldsymbol{H}}_\mathrm{aux}$ coincide for states with eigenenergies up to the cutoff energy E_c. In fact, using the tools proposed in [67] and with the strategy of [23], the following identity can be shown to hold true:

$$\begin{aligned}(e^{-i\hat{\boldsymbol{H}}_\mathrm{aux}t} - e^{-i\hat{\boldsymbol{H}}_N t})\hat{\mathbf{1}}_{(-\infty,E_\mathrm{c}]}(\hat{\boldsymbol{H}}_N) \\ = -ie^{-i\hat{\boldsymbol{H}}_\mathrm{aux}t}\int_0^t \mathrm{d}s e^{i\hat{\boldsymbol{H}}_\mathrm{aux}s}(\hat{\boldsymbol{H}}_\mathrm{aux} - \hat{\boldsymbol{H}}_N)e^{-i\hat{\boldsymbol{H}}_N s}\hat{\mathbf{1}}_{(-\infty,E_\mathrm{c}]} \\ = \mathcal{O}_0(\varepsilon^\infty|t|),\end{aligned} \tag{A6}$$

where $\hat{\mathbf{1}}_{(-\infty,E_\mathrm{c}]}$ is the spectral projection operator on energies below E_c.

Unfortunately, it is not possible to compare the dynamics generated by $\hat{\boldsymbol{H}}_\mathrm{aux}$ and the one generated by $\hat{\boldsymbol{H}}$ in the same manner, since the latter is an unbounded operator. We hence need to make a choice: Either we use the auxiliary Hamiltonian for the application of SAPT, which might, however, be a difficult task and which does not properly reflect the properties of the original Hamiltonian, or we remain with the original Hamiltonian and must therefore abandon any results on the convergence of the perturbation series. In this paper, we choose the second option.

APPENDIX B: EVALUATION OF THE OSCILLATOR HAMILTONIAN

The effective Hamilton operator of the oscillator model splits into the zeroth order contribution $\hat{\boldsymbol{h}}_{\mathrm{eff},0,\mathrm{p}}$ and a perturbation of second order, $\hat{\boldsymbol{h}}_{\mathrm{eff},2,\mathrm{p}}$. It is possible to compute the effect of the perturbative part of the Hamiltonian on the unperturbed spectrum $\{E_{d,\nu}\}_{d\in\mathbb{N}}$ by using standard quantum perturbation theory. The deviation of the spectrum due to $\hat{\boldsymbol{h}}_{\mathrm{eff},2,\mathrm{p}}$ results from computing the expectation value of $\hat{\boldsymbol{h}}_{\mathrm{eff},2,\mathrm{p}}$ in the unperturbed states $\{\Xi^0_{d,\nu}\}_{d\in\mathbb{N}}$, namely $\Delta E_{d,\nu} \coloneqq \langle \Xi^0_{d,\nu}, \hat{\boldsymbol{h}}_{\mathrm{eff},2,\mathrm{p}}\Xi^0_{d,\nu}\rangle_\mathrm{s}$. For notational reasons, we split the perturbation operator into two parts: A "kinetic" one $\boldsymbol{h}^\mathrm{kin}_{\mathrm{eff},2,\mathrm{p}}(q,p)$ which depends not only on q but also on the momentum p. And a "potential" contribution $\boldsymbol{h}^\mathrm{pot}_{\mathrm{eff},2,\mathrm{p}}(q)$ which solely depends on q. Since these operators act trivially on the light Hilbert space by projecting on the state ζ_ν via $\boldsymbol{\pi}_\mathrm{p}$, we omit the action on the light states and only consider the scalar functions $h^\mathrm{kin}_{\mathrm{eff},2,\mathrm{p}}(q,p)$ and $h^\mathrm{pot}_{\mathrm{eff},2,\mathrm{p}}(q)$ given by

$$h^\mathrm{kin}_{\mathrm{eff},2,\mathrm{p}}(q,p) \coloneqq -\frac{L^2(\nu+\frac{1}{2})}{2M^2\Omega_0}\cdot\frac{p^2q^2}{(L^2+q^2)^3}, \tag{B1}$$

$$h^\mathrm{pot}_{\mathrm{eff},2,\mathrm{p}}(q) \coloneqq \frac{\nu^2+\nu+1}{4M}\cdot\frac{q^2}{(L^2+q^2)^2}. \tag{B2}$$

The concrete evaluation of the potential operator $\hat{h}^\mathrm{pot}_{\mathrm{eff},2,\mathrm{p}}$ as an expectation value in one of the oscillator eigenfunctions $\Xi_{d,\nu}(q)$ is trivial as it only depends on q: In position representation, we only have to integrate its symbol $h^\mathrm{pot}_{\mathrm{eff},2,\mathrm{p}}(q)$ over $(\Xi_{d,\nu}\bar{\Xi}_{d,\nu})(q) = (\bar{\Xi}_{d,\nu})^2(q)$. The kinetic term can be treated by means of the Weyl quantization integral in analogy to the definition in Eq. (2), but for scalar-valued symbols. Thereby, the p-variables turn into derivatives of the remaining q-dependent part of $h^\mathrm{kin}_{\mathrm{eff},2,\mathrm{p}}$ and the eigenfunctions $\Xi_{d,\nu}(q)$. In order to simplify the analysis, we use partial integration to shift all the derivatives on the functions $\Xi_{d,\nu}(q)$. We introduce a new adapted coordinate $u_\nu \coloneqq \sqrt{M\Omega_\nu}q$ and the parameter $\ell_\nu \coloneqq \sqrt{M\Omega_\nu}L$. Eventually, we express the quantum oscillator solutions $\Xi_{d,\nu}(q)$ in terms of Hermite polynomials $\{H_d(u_\nu)\}_{d\in\mathbb{N}}$. Eventually, this gives for the expectation values

$$\Delta E^{\mathrm{pot}}_{d,\nu} = \frac{\Omega_\nu(\nu^2+\nu+1)}{4\sqrt{\pi}2^d d!}\int_{\mathbb{R}} e^{-u_\nu^2}\frac{u_\nu^2}{(\ell_\nu^2+u_\nu^2)^2}H_d^2(u_\nu)\mathrm{d}u_\nu,$$
$$\Delta E^{\mathrm{kin}}_{d,\nu} = -\frac{\ell_\nu^2\Omega_\nu^2(\nu+\frac{1}{2})}{4\sqrt{\pi}\Omega_0 2^d d!}\int_{\mathbb{R}} e^{-u_\nu^2}\frac{u_\nu^2}{(\ell_\nu^2+u_\nu^2)^3}[H_d^2(u_\nu)(u_\nu^2-2d-1)-d^2H_{d-1}^2(u_\nu)$$
$$-\frac{1}{4}H_{d+1}^2(u_\nu)+d\cdot H_{d-1}(u_\nu)H_{d+1}(u_\nu)]\mathrm{d}u_\nu. \tag{B3}$$

In order to solve the u_ν–integrals, we take advantage of the series representation of the Hermite polynomials,

$$H_d(u_\nu) = d!\sum_{m=0}^{\lfloor\frac{d}{2}\rfloor}\frac{(-1)^m}{m!(d-2m)!}(2u_\nu)^{d-2m}, \tag{B4}$$

to pull out the u_ν-dependence. The resulting integrals for the potential and the kinetic part have the form

$$I(\lambda) \coloneqq \int_{\mathbb{R}} e^{-u_\nu^2}\frac{u_\nu^{2\lambda}}{(\ell_\nu^2+u_\nu^2)^2}\mathrm{d}u_\nu,$$
$$J(\lambda) \coloneqq \int_{\mathbb{R}} e^{-u_\nu^2}\frac{u_\nu^{2\lambda}}{(\ell_\nu^2+u_\nu^2)^3}\mathrm{d}u_\nu, \tag{B5}$$

where λ is a parameter which changes according to the choice of d. It is possible to derive recursion relations for solving $I(\lambda)$ and $J(\lambda)$ for generic λ. The required input are the first few integrals, $I(0)$, $I(1)$, $J(0)$, $J(1)$, and $J(2)$ which can be solved by hand. For deriving the recursion relation, we add and subtract terms in the integral which sum up to zero but which allow one to reduce the integral to terms that depend on the preceding integrals. For example, the integral $I(\lambda)$ unfolds to

$$I(\lambda) = \Gamma\left(\lambda-\frac{3}{2}\right) - 2\ell_\nu^2 I(\lambda-1) - \ell_\nu^4 I(\lambda-2), \tag{B6}$$

where Γ is the standard gamma function. A similar relation for $J(\lambda)$ can be found by using the same trick. By introducing an appropriate recursion ansatz, it is possible to trace any $I(\lambda)$ back to $\Gamma(i)$ with $2\le i\le\lambda$, $I(1)$, and $I(0)$, and likewise for $J(\lambda)$ using $\Gamma(i)$ with $3\le i\le\lambda$, $J(2)$, $J(1)$, and $J(0)$. For the $I(\lambda)$'s, we employ

$$I(\lambda) \coloneqq a(\lambda)I(0) + b(\lambda)I(1) + \sum_{i=2}^{\lambda} c_i(\lambda)\Gamma\left(i-\frac{3}{2}\right) \tag{B7}$$

in Eq. (B6), and we determine the coefficients to

$$a(\lambda) = (1-\lambda)(-1)^\lambda \ell_\nu^{2\lambda}, \tag{B8}$$

$$b(\lambda) = \lambda(-1)^{\lambda-1}\ell_\nu^{2(\lambda-1)}, \tag{B9}$$

$$c_i(\lambda) = (1+\lambda-i)(-1)^{\lambda-i}\ell_\nu^{2(\lambda-i)}. \tag{B10}$$

Again, the same method applies to $J(\lambda)$. With these prerequisites, it is possible to determine $\Delta E_{d,\nu} = \Delta E^{\mathrm{kin}}_{d,\nu} + \Delta E^{\mathrm{pot}}_{d,\nu}$ for any d and ν in $\mathbb{N}$. To illustrate, the energy shift due to the potential term has the form

$$\Delta E^{\mathrm{pot}}_{d,\nu} = \frac{\Omega_\nu 2^d d!(\nu^2+\nu+1)}{4\hbar\sqrt{\pi}}\sum_{m=0}^{\lfloor\frac{d}{2}\rfloor}\sum_{k=0}^{\lfloor\frac{d}{2}\rfloor}$$
$$\times\frac{(-1)^{m+k}2^{-2(m+k)}}{m!k!(d-2m)!(d-2k)!}I(d-m-k+1), \tag{B11}$$

and likewise for the kinetic term but lengthier. By evaluating the sums and employing the specific $I(\lambda)$'s for every summand, we obtain the correct energy shift. Namely, the energy shifts for $d=0$ and $d=1$ are given by

$$\Delta E_{0,\nu} = \frac{\Omega_\nu(\nu^2+\nu+1)}{4\sqrt{\pi}}I(1) + \frac{\ell_\nu^2\Omega_\nu^2(\nu+\frac{1}{2})}{4\sqrt{\pi}\Omega_0}(2J(1)-J(2)),$$
$$\Delta E_{1,\nu} = -\frac{\Omega_\nu(\nu^2+\nu+1)}{2\sqrt{\pi}}(\sqrt{\pi}+2\ell_\nu^2 I(1)+\ell_\nu^4 I(0))$$
$$+\frac{\ell_\nu^2\Omega_\nu^2(\nu+\frac{1}{2})}{2\sqrt{\pi}\Omega_0}(J(1)+J(2)), \tag{B12}$$

with the integrals given by

$$I(0) = \frac{\sqrt{\pi}}{\ell_\nu^2} + \frac{\pi}{2\ell_\nu^3}e^{\ell_\nu^2}(2\ell_\nu^2-1)(\mathrm{erf}(\ell_\nu)-1), \tag{B13}$$

$$I(1) = -\sqrt{\pi} - \frac{\pi}{2\ell_\nu}e^{\ell_\nu^2}(1+2\ell_\nu^2)(\mathrm{erf}(\ell_\nu)-1), \tag{B14}$$

$$J(1) = \frac{\sqrt{\pi}}{4\ell_\nu^2}(1+2\ell_\nu^2) + \frac{\pi}{8\ell_\nu^3}e^{\ell_\nu^2}(1-4\ell_\nu^2-4\ell_\nu^4)(1-\mathrm{erf}(\ell_\nu)), \tag{B15}$$

$$J(2) = -\frac{\sqrt{\pi}}{4}(5+2\ell_\nu^2)$$
$$+\frac{\pi}{8\ell_\nu}e^{\ell_\nu^2}(3+12\ell_\nu^2+4\ell_\nu^4)(1-\mathrm{erf}(\ell_\nu)). \tag{B16}$$

Here, "erf" denotes the error function. Employing the integrals in the above equations yields the expressions in Eq. (44).

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