Quantum Cosmological Backreactions I: Cosmological Space Adiabatic Perturbation Theory

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Abstract

The search for quantum gravity fingerprints in currently available cosmological data that have their origin from the Planck era is of growing interest due to major recent progress both in the theoretical modelling as well as the observational precision. Unsurprisingly, the theoretical predictions are very sensitive to the quantum effects that occur close to the classical big bang singularity. It is therefore of substantial interest to describe these effects as precisely as possible.

This is the first in a series of papers that aim at improving on the treatment of quantum effects that arise due to backreactions between matter and geometry. The technique we employ is space adiabatic perturbation theory (SAPT) in the form developed in seminal papers by Panati, Spohn and Teufel. SAPT is a generalisation of the more familiar Born Oppenheimer Approximation (BOA) that applies well in systems that allow a split of the degrees of freedom into two sets that propagate on rather different time scales such as the homogeneous and inhomogeneous field modes in cosmology. We will show that this leads to presently neglected correction terms in the quantum Friedman equations.

In the present paper we adapt and generalise SAPT to the hybrid approach to quantum cosmology developed by Mena Marugan et al. that allows for a systematic quantum separation of the (in)homogeneous modes. Since SAPT was developed for quantum mechanics rather than quantum field theory, several challenges have to be met.

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1 Introduction

Physical systems often display a separation of time scales which can be exploited when solving the equations governing them. The historically first example was the approximate solution of the spectral problem for molecules introduced by Born and Oppenheimer [1] henceforth called Born Oppenheimer approximation (BOA). Here the slow degrees of freedom are the nuclear ones while the fast degrees of freedom are those of the electrons owing to a mass ratio of about 2000 or more. Intuitively then the electrons "adiabatically" adapt their fast motion to the slow motion of the nuclear degrees of freedom without much disturbance.

In the leading order of that mass ratio, one neglects the modifications that the nuclear part of the Hamiltonian has on the eigenstates of the electrons which parametrically depend on the location of the nuclear degrees of freedom. This allows for an approximate solution of the full spectral problem in that one finds an effective Hamiltonian for the nuclear degrees of freedom on a subspace of the full Hilbert space labelled by an eigenvalue of the electronic part of the Hamiltonian leading to the energy bands of the coupled system. However, when one tries to go beyond that leading order and tries to incorporate backreaction effects, one is confronted with an infinite set of coupled equations labelled by the undisturbed energy eigenvalues of the electrons which in contrast to the leading order is not solvable exactly in practice.

One way to view space adiabatic perturbation theory (SAPT), developed in particular by Panati, Spohn and Teufel (see [2] and references therein), is to consider it to be as a systematic approach to perturbatively decouple this infinite set of equations. Namely, the backreaction mixes the undisturbed electronic energy eigenstates and the exact effective Hamiltonian acts on a subspace of the Hilbert space which is rotated as compared to the undisturbed subspace labelled by the energy band parameter. SAPT provides a systematic perturbative construction, for each energy level of the unperturbed fast part of the Hamiltonian, of i. the projection onto the corresponding subspace, ii. the unitary rotation between that subspace and the undisturbed one and iii. the effective slow Hamiltonian acting on that subspace. Being a perturbation series, the corresponding operators can be truncated at the desired level of precision.

This "space" adiabatic scheme, that we just described, includes the "time" adiabatic one (see e.g. [3]) which was developed for explicitly time dependent Hamiltonians, where the external time scale is much larger than the internal one, in the following sense: We can pass to the extended phase space formalism and treat time as a dynamical "spatial" degree of freedom if we impose the constraint that the sum of Hamiltonian and momentum conjugate to time is vanishing. As such, SAPT is already well adapted to generally covariant systems that have no Hamiltonian but rather a Hamiltonian constraint as it happens in quantum gravity and more specifically quantum comsmology.

In this series of papers we thus advocate to further develop the work of [4] and employ SAPT for quantum cosmology, in particular quantum cosmological perturbation theory (QCPT). To make the presentation as clear as possible, we consider as matter content just an inflaton field (and possibly Gaussian dust as a dynamical clock, see [5, 6] and references therein) but our formalism can be easily extended to more complicated models. To see how SAPT can be applied, note that in cosmological perturbation theory one splits the field degrees of freedom into a dominant, homogeneous contribution and an inhomogeneous perturbation thereof [7]. The corresponding perturbation series in principle involves all orders, but already the second order is non trivial and we confine ourselves to second order in this series of papers. In particular, it makes a crucial difference whether one considers the homogeneous sector as a background or not. In either case one must deal with the issue of gauge invariance with respect to the perturbative fragment of the spacetime diffeomorphism group. In the background approach, which by definition neglects backreaction effects, one considers only the inhomogeneous degrees of freedom as dynamical and in the quantum theory thus effectively conducts quantum field theory on the given background spacetime [8] (QFT in CST), albeit in terms of the corresponding gauge invariant field modes (e.g. Mukhanov-Sasaki field [7] if there is no dust present).

If one wants to treat the homogeneous degrees of freedom as dynamical and thus allows for backreaction effects then in particular the constraint analysis must be properly adapted to extract the correct gauge invariant degrees of freedom. To the best of our knowledge, this clasiscal programme has been carried out for the first time (to second order) in [9] and we will adopt it for our purposes. In particular it is important to carry out a canonical transformation (to second order) on the *full phase space* in order that the constraints still form a first class system (to second order). Simultaneously that transformation must be chosen in such a way, that the second order contribution to the Hamiltonian (constraint) can be represented on an appropriate Hilbert space.

When quantising the complete system, i.e. homogeneous and inhomogeneous degrees of freedom, one has the freedom to choose different types of Hilbert space representations for these two sets of variables. This is the idea of the $hybrid\ LQC$ quantisation [9]: Here the perturbations are represented on suitable Fock spaces, thus taking advantage of their at most quadratic appearance in the Hamiltonian constraint, while the homogeneous degrees of freedom are quantised by using Loop Qauntum Cosmology (LQC) [10] techniques. Here LQC is a mini supersapce quantisation of just the homogeneous degrees of freedom using techniques from Loop Quantum Gravity (LQG) [11] which is a candidate theory for full quantum gravity. The LQC representation is well adapted to the non-polymnomial appearance of the homogeneous degrees of freedom in the Hamiltonian (constraint). In this series of papers we will adopt parts of the hybrid LQC idea but we will consider different possibilities concerning the quantisation of the homogeneous sector.

The current ideas, mostly within the LQC scenario, to describe the interaction between homogeneous and inhomogeneoeus degrees of freedom include: 1. the dressed metric approach [12], 2. the rainbow metric approach [13], the 3. the deformed algebra approach [14] and the hybrid approach [9]. In the dressed metric approach, for full LQG proposed for the first time in [15], one computes the partial expectation values of the Hamiltonian (constraint) with respect to a semiclassical state of the homogeneous sector and then derives the free QFT in CST on the resulting background spacetime. The dynamics of the background is chosen to be derived from the expectation value of the homogeneous contribution to the Hamiltonian constraint with respect to that semiclassical state (including quantum corrections from fluctuations and those that come from the particular LQC quantisation method), leading to the so called effective equations. In the rainbow metric approach one similarly takes such a partial expectation value and then recasts the resulting effective metric, separately for each term of the Hamiltonian (constraint) labelled by a mode number, into a FRW form thereby making scale factor and lapse function depending on that mode number (hence the name rainbow). As far as the quantisation of the inhomogeneous sector is concrened, both of these approaches are equivalent. In the deformed algebra approach one requires that the constraints up to second order in the inhomogneities close (up to second order) in the sense of Poisson brackets when one replaces the background variables by effective functions thereof. This can be considered as a different method to choose the semiclassical state although it is not clear that a semiclassical state exists which reproduces all the coefficients needed for such a closure. Finally, in the hybrid approach, one assumes that certain quantum states for the homogeneous sector exist such that the full quantum constraint including second order inhomogenous contributions can be recast into a Schrödinger type first order equation with respect to the homogenous inflaton mode considered as an internal time. The list of assumptions include that second order derivatives with respect to internal time can be neglected and the validity of an Ansatz for the wave functions of Born-Oppenheimer type.

To the best of our understanding, these methods do not incorporate backreaction effects in the same sense as the zeroth order of the BOA does not include them. Also, to the best of our understanding, the various assumptions that went into these approximations are not easy to control. Accordingly, it is an important question how one can improve on this. In this series of papers we would like to convince the reader that SAPT methods are a powerful tool for achieving just that. SAPT follows an iterative systematic algorithm that can be applied as easily as standard quantum mechanical stationary perturbation theory can be, although concrete calculations become quickly involved and tedious as we increase the adiabatic order. The basic idea is that the homogeneous modes can be considered as the slow degrees of freedom while the inhomogeneous ones play the role of the fast degrees of freedom. Roughly this happens because the homogeneous mode, being the integral (or sum) over the inhomogeneous modes, is a kind of centre of mass mode with respect to

the inhomogeneous ones and as in classical mechanics comes with the large total mass of the system rather than the small individual ones. This will be explained in later parts of this paper. Accordingly the SAPT scheme should be quite appropriate for the hybrid treatment suggested in [9].

However, the application of the SAPT scheme to quantum cosmology is not entirely straightforward. We meet the following challenges:

i.

SAPT was developed for systems with a finite number of degrees of freedom while we are interested in quantum field theory. Hence, rather innocent looking assumptions of the SAPT scheme such as that the Hilbert space can be considered as a tensor product of a fast and slow Hilbert space are no longer granted to make any sense as was first remarked in [4].

ii.

Furthermore, many of the theorems proved in [2] rely on the assumption of dealing with everywhere smooth symbol classes of fast Hilbert space operator valued functions on the slow phase space which is not the case in our applications. Accordinly we will not have much to say about the convergence of the perturbation series (in terms of the adiabatic parameter) and we leave that part of the analysis for future research.

iii.

In contrast to BOA, in SAPT one is able to to deal with situations where the part of the Hamiltonian that describes the fast degrees of freedom depends on both configuration and momentum variables of the slow sector. This is important for quantum cosmology since for instance the Mukhanov-Sasaki mass term has precisely this property and thus requires the full $Weyl\ quantisation\ technology$ of the SAPT scheme.

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Unfortunately, the mass squared terms that appear in quantum cosmology not only depend on negative powers of the configuration degrees of freedom of the homogeneous sector but also on the momenta. Even worse, they are not positive definite. This raises complicated domain issues both in the inhomogeneous QFT sector as well as in the homogeneous QM sector. In the QFT sector it begs the question of how to treat quantum fields with varying indefinite mass squared terms and in the QM sector one meets rather non-polynmial operators usually not discussed in QM and whose degree of non-polynomiality exceeds even the situation one meets in LQC.

We also should comment on the physical intution of the adiabatic scheme, which is different for systems with Hamiltonian constraints and a true Hamiltonian respectively. In the more familiar latter case, the physical argument is based on 1. the equipartition theorem [17], 2. the ergodicity assumption and 3. the assumption that the Hamiltonian is of second order in the momenta. In that case the time average, which due to ergodicity equals the phase space average in say the canonical ensemble, of the kinetic terms in the Hamiltonian are all equal implying that the light degrees of freedom in average are much faster than the heavy ones. That intuition fails when we have a Hamiltonian constraint. However, in this case the constraint itself dictatates that the kinetic term of the slow mode is equal to the sum of the kinetic terms of the fast modes which at least in the kinetic energy dominated regime of tyhe phase space leads to the same conclusion if the number of fast modes is much smaller than the inverse square of the adiabatic parameter. In a quantum mechanical system that latter number is finite by itself in absolute terms, in the quantum field theory case it is effectively finite in any Fock state which only contains finitely many excitations and the reasoning will apply at least to the lower lying excited states.

On the other hand, technically speaking, the SAPT scheme works as soon as the system involves an adiabatic parameter that multiplies the momenta of the "slow" degrees of frteedom.

The architecture of this paper is as follows:

In section two we will derive the SAPT programme in a self-contained fashion for the case of a finite dimensional phase space. This also serves to introduce a simple notation aiming at highest

possible transpararency.

In section three we will address the conceptual and mathematical complications when applying SAPT to quantum cosmology and their possible solutions, thus preparing the ground for the remaining papers of this series.

In section four we summarise and give an outlook to the applications discussed in the other papers of this series.

2 Elements of Space Adiabatic Perturbation Theory (SAPT)

In the first subsection we explain our notation and the basic ideas underlying the SAPT scheme. That notation is simplified as compared to the more technical subsequent papers of this series in order to be able to better focus on the underlying ideas. In the second subsection we derive the essential inductive formulae underlying the adiabatic expansion. As mentioned before, we will not discuss the sense of convergence of the adiabatic perturbation series. This can be done by introducing notions from the theory of pseudo differential operators called symbol classes for which we refer the interested reader to [2].

2.1 Notation and basic idea

Throughout this section we only consider finite dimensional phase spaces. To avoid unnecessary cluttering of formulae, it will in fact be sufficient to consider a four dimensional phase space, the generalisation to higher dimensional ones being straightworward and obvious. To a certain extent it is also possible to generalise this to finite dimensional phase spaces which are not vector specs [4]. The present phase space is thus coordinatised by a "slow" canonical pair z=(q,p) and a fast canonical pair (x,y) with standard canonical brackets $\{p,q\}=\{y,x\}=1$, all others vanishing. The dimensionfree adiabatic parameter will be denoted by ϵ . We denote the trivially rescaled slow momentum by $p':=\epsilon p$ and accordingly z'=(q,p'). A basic assumption is that the Hamiltonian (constraint) of the system can be written in the form

$$h(q, p, x, y) = h_0((q, p', x, y; \epsilon) + \epsilon^r h_1(q, p', x, y; \epsilon)$$
(2.1)

The term h_1 is allowed to vanish while h_0 never vanishes. If h_1 is non-vanishing we have $r \in \mathbb{N} - \{0\}$ and both h_0, h_1 are polynomials in ϵ of finite degree with coefficients independent of ϵ where the coefficients of zeroth order are non-vanishing. The form (2.1) can often be obtained by multiplying the original Hamiltonian by a sufficiently high power of ϵ in which case the spectrum of (2.1) has to be rescaled by the corresponding inverse power, after the perturative computation has been completed. Furtheremore, the piece h_0 of the Hamiltonian comprises all terms of h which upon quantisation of just the fast degrees of freedom allows for an easy diagonalisation on the Hilbert space \mathcal{H}_f of the fast degrees of freedom for all parameter values of q,p'. Note that this means that any term of the form $\epsilon^s f(q,p')$, $n\geq 0$ in the classical Hamiltonian which is independent of x,y will be subsumed under h_0 since the quantisation on \mathcal{H}_f yields the trivial symbol $\epsilon^s f(q,p')1_s$ and shifts the spectrum of $h_0(q,p')$ by $\epsilon^n f(q,p')$. This is in contrast to the BOA which would treat such a term as of higher order if either n>0 or $f(q,p')=\epsilon^l f(q,p)$, l>0.

Turning to the quantisation, we represent the "slow" degrees of freedom as operators $Q,P'=\epsilon P$ on the Hilbert space $\mathcal{H}_s=L_2(\mathbb{R},dq)$ and the fast degrees of freedom as operators X,Y on the Hilbert space $\mathcal{H}_f=L_2(\mathbb{R},dx)$. The full Hilbert space is the tensor product Hilbert space $\mathcal{H}_f\otimes\mathcal{H}_s$ on which x acts as $X\otimes 1_s$ and q as $1_f\otimes Q$ respectively etc.

We will also be dealing with so-called symbols. These are functions on the slow phase space with values in the set of linear operators on \mathcal{H}_f . We will assume that all symbols that we encounter have a common, invariant and dense domain for all q,p' and are smooth in q,p'. This turns out to be the case in our applications as the symbols that we encounter are either those corresponding to (2.1) or originate from the eigenfunctions $e_{n,a}(z')$ discussed below which both have the required properties.

Intuitively, a symbol $(q,p')\mapsto f(q,p')$ can be considered as arising from a function f(q,p',x,y) on the full phase space by just quantising the fast sector and choosing some operator ordering to obtain f(q,p')=f(q,p',X,Y). Unless confusion may arise, we will denote symbols and their underlying phase space functions by the same $lower\ case\ letter\ f$.

The next ingredient will be the Weyl quantisation F:=W(f) of a symbol. We will denote Weyl quantisations by $capital\ letters\ F$. These are now operators on the total product Hilbert space and in case that f deopends polynomially on p' then F is just the symmetric ordering of the formal expression f(Q,P'). To be clear, the Weyl quantisation and the associated $Moyal\ product$ is here with respect to the $rescaled\ Planck\ constant\ \hbar':=\epsilon\hbar$. This arises because of the commutation relations $[P',Q]=i\hbar'1_s$ naturally as follows:

The Weyl elements are defined by

$$W(k,l) := \exp(i\frac{k Q + lP'}{\hbar'}) \tag{2.2}$$

and the Weyl quantisation of a symbol f by

$$W(f) := \int_{\mathbb{R}^2} \frac{dk \, dl}{[2\pi\hbar']^2} \, \hat{f}(k,l) \otimes W(k,l) \tag{2.3}$$

where \hat{f} denotes the Fourier transform of the symbol f

$$\hat{f}(k,l) = \int_{\mathbb{R}^2} dq \, dp' \, \exp\left(-i\frac{kq + lp'}{\hbar'}\right) f(q,p') \tag{2.4}$$

Note that k, l have the dual dimension of q, p' so that the products kq, lp' have the dimension of \hbar . Then it is well known that for two symbols f, g we have the $Moyal\ product$ formula

$$W(f) W(g) = W(f * g), (f * g)(q, p') := \left[\exp(\frac{i\hbar'}{2}\theta_{12}) \cdot f(q_1, p'_1) g(q_2, p'_2)\right]_{q_1 = q_2 = q, p'_1 = p'_2 = p'}$$

$$\theta_{12} := \frac{\partial^2}{\partial p'_1 \partial q_2} - \frac{\partial^2}{\partial p'_2 \partial q_1}$$
(2.5)

The Moyal product is associative but not commutative. Note that in the Moyal commutator

$$[f,g]_* = f * g - g_* f = [f,g] + O(\hbar')$$
(2.6)

the term [f,g]=f g-g f of zeroth order in \hbar' which is just the usual commutator of symbols is not vanishing in general in contrast to the classical case of Weyl quantisation on just \mathcal{H}_s .

Weyl quantisation thus serves several purposes at the same time: First it allows us to write any operator on the full Hilbert space $\mathcal{H}_f \otimes \mathcal{H}_s$ in the form of a slow phase space integral of elementary operators of the form $A_f(z) \otimes B_s(z)$ thus allowing us to simplify its spectral problem when the spectral problem of the $A_f(z)$ is known in closed form. Secondly, the Moyal product allows for a systematic power expansion in terms of the adiabatic parameter ϵ and thus enables us to set up a perturbative diagonalisation scheme. This follows from the fact that $W(f)W(g)-W(fg)=W(f*g-fg)=O(\epsilon)$.

Thus in what follows we will assume that the spectral problem of the symbols

$$h_0(z) := h_0(z, X, Y; \epsilon) \tag{2.7}$$

is known in closed form. In our applications the spectra will turn out to be pure point with eigenvalues $E_n(z'), n \in \mathbb{N}$ and an orthonormal basis of eigenfunctions $e_{n,a}(z'), a=1,...,d_n$ where $d_n \in \mathbb{N}$ denotes its degeneracy which we assume to be a constant in z'. An important assumption is the absence of eigenvalue crossing, that is, $E_m(z') - E_n(z') \neq 0$ for all $z', m \neq n$. To get strong mathematical results one may impose the stronger $gap\ condition\ g_n := \inf_{z,m\neq n} |E_m(z') - E_n(z')| > 0$ (not necessarily uniform in n) [2]. What happens when these conditions for some n are violated in

certain submanifolds of the slow phase space is an interesting question¹ which has to be considered in a case by case analysis.

The next building blocks of the SAPT scheme are the spectral projection symbols

$$\pi_{n,0}(z') := \sum_{a=1}^{d_n} e_{n,a}(z') < e_{n,a}(z'), >_{\mathcal{H}_f}$$
(2.8)

and the unitary symbols

$$u_{n,0}(z') := \sum_{n \in \mathbb{N}} \sum_{a=1}^{d_n} b_{n,a} < e_{n,a}(z'), .>_{\mathcal{H}_f}$$
 (2.9)

where $b_{n,a}$ is any orthormal basis of \mathcal{H}_f . The important point is that the reference vectors $b_{n,a}$ do not depend on z' and we can pick them conveniently according to the concrete physical application, e.g. $b_{n,a} := e_{n,a}(z'=0)$. With their help we can define the reference projection

$$r_n := \sum_{a=1}^{d_n} b_{n,a} < b_{n,a}, .>_{\mathcal{H}_f}$$
 (2.10)

The technical relevance of this $reference\ structure$ is that r_n in contrast to $\pi_{n,0}$ does not receive adiabatic corrections throughout the application of the SAPT scheme and thus always defines an $exact\ projector$

$$R_n = W(r_n) = r_n \otimes 1_s \tag{2.11}$$

which will be crucial for the adiabatic expansion and its spectral analysis. Note also that $u_{n,0}=u_0$ is in fact independent of n while its adiabatic corrections will depend on n. In general we have series expansions

$$\pi_n(z') = \lim_{N \to \infty} \pi_{n,N}(z'), \ \pi_{n,N}(z') = \sum_{k=0}^{N} \epsilon^k \ \pi_n^{(k)}(z'), \ \pi_n^{(0)}(z') = \pi_{n,0}(z')$$

$$u_n(z') = \lim_{N \to \infty} u_{n,N}(z'), \ u_{n,N}(z') = \sum_{k=0}^{N} \epsilon^k \ u_n^{(k)}(z'), \ u_n^{(0)}(z') = u_{n,0}(z')$$
(2.12)

where the $\pi_{n,N}$, $u_{n,N}$ are approximate Moyal projections and Moyal unitarities up to corrections of order ϵ^{N+1} , see below. Due to the linearity of the Weyl map we have

$$\Pi_{n} := W(\pi_{n}), \ \Pi_{n,N} := W(\pi_{n,N}), \ \Pi_{n}^{(k)} := W(\pi_{n}^{(k)}),
U_{n} := W(u_{n}), \ U_{n,N} := W(u_{n,N}), \ U_{n}^{(k)} := W(u_{n}^{(k)})
\Pi_{n} = \lim_{N \to \infty} \Pi_{n,N}, \ \Pi_{n,N} = \sum_{k=0}^{N} \epsilon^{k} \Pi_{n}^{(k)}
U_{n} = \lim_{N \to \infty} U_{n,N}, \ U_{n,N} = \sum_{k=0}^{N} \epsilon^{k} U_{n}^{(k)}$$
(2.13)

As we will spell out in detail below, the operators $\Pi_{n,N}:=W(\pi_{n,N}),\ U_{n,N}:=W(u_{n,N})$ will be constructed in such a way that the operator $U_{n,N}$ H $U_{n,N}^{\dagger},\ H=W(h)$ preserves the subspace $R_n\mathcal{H}$ up to corrections of order ϵ^{N+1} . It thus coincides there up corrections of order ϵ^{N+1} with the operator $H_{n,N}=R_nU_{n,N}HU_{n,N}^{\dagger}R_n$ on the Hilbert subspace $R_n\mathcal{H}\cong\mathbb{C}^{d_n}\otimes\mathcal{H}_s$. The importance

¹In molecular physics this leads to a rearrangement of the orbital binding sructure of atoms and can be observed e.g. in organic molecules where the process is called isomerization.

of the reference structure now becomes manifest: While we have $H_{n,N}=U_{n,N}\tilde{H}_{n,N}U_{n,N}^{\dagger}$ up to corrections of order ϵ^{N+1} where $\tilde{H}_{n,}=\Pi_{n,N}H\Pi_{n,N}$, since $\Pi_{n,N}$ is not an exact projector, the perhaps more natural operator $\tilde{H}_{n,N}$ which would not involve the objects $U_{n,N}$ does not preserve the subspace $\Pi_{n,N}\mathcal{H}$. Hence while the spectral analysis of $H_{n,N}$ on $R_n\mathcal{H}$ can be preformed in the standard way, it would be unclear how to do that for $\tilde{H}_{n,N}$ on $\Pi_{n,N}\mathcal{H}$. Note that the problem is worse than $\tilde{H}_{n,N}$ not preserving its domain $within\ \Pi_{n,N}|calH$, it actually maps its domain outside of $\Pi_{n,N}\mathcal{H}$.

This is then the perturbative $adiabatic\ decoupling$ that we wanted to achieve. The spectrum of $H_{n,N}$, denoted by $E_{n,N}$ is referrred to as the n-th $energy\ band$. If $f_{n,N}\in R_n\mathcal{H}$ is a generalised eigenvector of $H_{n,N}$ with eigenvalue λ then up to corrections of order ϵ^{N+1} the vector $\tilde{f}_{n,N}=U_{n,N}^{\dagger}f_{n,N}$ is a generalised eigenvector of H with the same eigenvalue since (we drop the $O(\epsilon^{N+1})$ terms)

$$H\tilde{f}_{n,N} = HU_{n,N}^{\dagger} R_n U_{n,N} U_{n,N}^{\dagger} f_{n,N} = H\Pi_{n,N} U_{n,N}^{\dagger} f_{n,N} = \Pi_{n,N} HU_{n,N}^{\dagger} f_{n,N}$$

$$= U_{n,N}^{\dagger} (R_n U_{n,N} HU_{n,N}^{\dagger} R_n) f_{n,N} = U_{n,N}^{\dagger} H_{n,N} f_{n,N} = \lambda \tilde{f}_{n,N}$$
(2.14)

The approximate eigenvector $\tilde{f}_{n,N}$ is an element of the approximately invariant subspace $\Pi_{n,N}\mathcal{H}$ up to corrections of order $O(\epsilon^{N+1})$ because (we again drop the corrections)

$$\tilde{f}_{n,N} = U_{n,N}^{\dagger} R_n U_{n,N} U_{n,N}^{\dagger} f_{n,N} = \Pi_{n,N} \tilde{f}_{n,N}$$
(2.15)

In this way the $U_{n,N}$ are displayed as an auxiliary structure introduced in order to solve the spectral problem including backreation but they have no further fundamental relevance as is also clear from the fact that they are not uniquely determined by the perturbative scheme in contrast to the $\Pi_{n,N}$. In particular, the $U_{n,N}$ are not to be confused with the unitary map V that maps $\mathcal H$ to $L_2(\sigma(H),d\mu)$, granted to exist by the spectral theorem, where $\sigma(H)$ is the spectrum of H and μ its spectral measure (in that Hilbert space, H is a multiplication operator). This is already clear from the fact that $U_{n,N}$ generically depends on n while V does not.

The fact that the $\Pi_{n,N}$ approximately commute with H and are approximate projections displays them as approximants of spectral projections of H on the part $E_{n,N}$ of the spectrum. The spectral projections are of course not necessarily mutually orthogonal even if the gap condition holds (for instance, h(z') could have pure point spectrum but H could have absolutely continuous spectrum), unless the energy bands are mutually disjoint.

We proceed to detail the perturbative analysis.

2.2 Perturbative Construction

The objective of the construction is to compute the set of operators

$$\Pi_n := W(\pi_n), \ U_n := W(u_n), \ H := W(h), \ R_n = W(r_n) = r_n \otimes 1_s$$
 (2.16)

such that the following relations hold:

$$\Pi_n^2 - \Pi_n = \Pi_n^{\dagger} - \Pi_n = [\Pi_n, H] = U_n U_n^{\dagger} - 1_{\mathcal{H}} = U_n^{\dagger} U_n - 1_{\mathcal{H}} = U_n \Pi_n U_n^{\dagger} - R_n = 0$$
 (2.17)

Here $(.)^{\dagger}$ denotes the adjoint on $\mathcal{H}_f \otimes \mathcal{H}_s$. Using the properties of Weyl quantisation this will be granted by the corresponding symbol relations

$$\pi_n * \pi_n - \pi_n = \pi_n^{\dagger} - \pi_n = \pi_n * h - h * \pi_n = u_n * u_n^{\dagger} - 1_f = u_n^{\dagger} * u_n - 1_f = u_n * \pi_n * u_n^{\dagger} - r_n = 0$$
 (2.18)

Here $(.)^{\dagger}$ denotes the adjoint on \mathcal{H}_f and it should be clear from the lower case and upper case letter notation which adjoint is being taken.

To obtain the π_n, u_n define $\pi_{n,0}, u_{n,0}$ as in (2.8), (2.9) and expand as in (2.12). The symbols $\pi_n^{(k)}, u_n^{(k)}$ for k>0 are now defined inductively by requiring the approximate relations

$$\pi_{n,N} * \pi_{n,N} - \pi_{n,N} = \pi_{n,N}^{\dagger} - \pi_{n,N} = \pi_{n,N} * h - h * \pi_{n,N} = u_{n,N} * u_{n,N}^{\dagger} - 1_f$$

$$= u_{n,N}^{\dagger} * u_{n,N} - 1_f = u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} - r_n = O(\epsilon^{N+1})$$
(2.19)

where $O(\epsilon^{N+1})$ is a symbol whose leading order in its ϵ expansion is ϵ^{N+1} or higher. Since for any two symbols a,b we have $a*b=ab+O(\epsilon)$ we note that (2.19) is certainly satisfied for N=0 since

$$\pi_{n,0}\pi_{n,N} - \pi_{n,0} = \pi_{n,0}^{\dagger} - \pi_{n,0} = [\pi_{n,0}, h_0] = u_{n,0}u_{n,0}^{\dagger} - 1_f = u_{n,0}^{\dagger} * u_{n,0} - 1_f = u_{n,0}\pi_{n,0} * u_{n,0}^{\dagger} - r_n = 0$$
(2.20)

and we used $[a,h]=[a,h_0]+O(\epsilon)$ for any symbol a. Actually, the construction only grants that in this way we obtain (2.18) but with zero replaced by $O(\epsilon^{\infty})$ (e.g. $e^{-1/\epsilon}$). In [2] resolvent methods are used to actually substitute $O(\epsilon^{\infty})$ exactly by zero but for our purposes finite order approximations will be sufficient.

Also note that we do not impose any conditions on $O(\epsilon^{N+1})$. In the ideal scenario we would like it to be of the form $\epsilon^{N+1}f(z')$ where f(z') is a bounded operator on \mathcal{H}_f with bound ||f(z')|| perhaps even uniform on the slow phase space. We refer to [2] for circumstances under which one gets such results, however, these do not apply here and we confine ourselves to a formal power expansion.

We will now inductively construct first $\pi_{n,N}$ and after that $u_{n,N}$.

2.2.1 Construction of the Moyal projections

We will see that it is possible to construct all $\pi_n^{(k)}$ such that $(\pi_n^{(k)})^\dagger = \pi_n^{(k)}$ exactly for all k thus implying

$$)\pi_{n,N}^{\dagger} = \pi_{n,N}, \ \Pi_{n,N}^{\dagger} = \Pi_{n,N}$$
 (2.21)

exactly for all N which is included in our set of induction assumptions.

We isolate the leading order contributions

$$\pi_{n,N} * \pi_{n,N} - \pi_{n,N} =: a_{n,N} \epsilon^{N+1} + O(\epsilon^{N+2}), \quad \pi_{n,N} * h - h * \pi_{n,N} =: b_{n,N} \epsilon^{N+1} + O(\epsilon^{N+2})$$
 (2.22)

The symbols $a_{n,N}, b_{n,N}$ are symmetric and antisymmetric operators on \mathcal{H}_f respectively due to the Moyal identity for symbols f, g

$$(f * g)^{\dagger} = g^{\dagger} * f^{\dagger} \tag{2.23}$$

We obtain

$$\pi_{n,N+1} * \pi_{n,N+1} - \pi_{n,N+1}$$

$$= \pi_{n,N} * \pi_{n,N} - \pi_{n,N} + \epsilon^{N+1} \{ [\pi_n^{(N+1)} * \pi_{n,N} + \pi_{n,N} * \pi_n^{(N+1)} * -\pi_n^{(N+1)} \} + \epsilon^{2(N+1)} \pi_n^{(N+1)} * \pi_n^{(N+1)} \}$$

$$= \epsilon^{N+1} \{ a_{n,N} + \pi_n^{(N+1)} \pi_n^{(0)} + \pi_n^{(0)} \pi_n^{(N+1)} - \pi_n^{(N+1)} \} + O(\epsilon^{(N+2)}$$
(2.24)

We conclude

$$-a_{n,N} = \pi_n^{(N+1)} \pi_n^{(0)} + \pi_n^{(0)} \pi_n^{(N+1)} - \pi_n^{(N+1)}$$
(2.25)

Since we will it frequently let us abbreviate

$$P_n = \pi_{n,0}, \ P_n^{\perp} = 1_{\mathcal{H}_f} - P_n$$
 (2.26)

Then by projecting (2.25) to the block diagonal pieces

$$-P_n a_{n,N} P_n = P_n \pi_n^{(N+1)} P_n, \quad P_n^{\perp} a_{n,N} P_n^{\perp} = P_n^{\perp} \pi_n^{(N+1)} P_n^{\perp}$$
 (2.27)

while for the projection to the off block diagonal pieces we obtain the consistency condition

$$P_n a_{n,N} P_n^{\perp} = P_n^{\perp} a_{n,N} P_n = 0 (2.28)$$

This identity follows from the defining equation (2.22) which we project to the off block diagonal pieces

$$\epsilon^{N+1} P_n a_{n,N} P_n^{\perp} = P_n (\pi_{n,N} * \pi_{n,N} - \pi_{n,N}) P_n^{\perp} + O(\epsilon^{N+2})
= \pi_{n,N} (\pi_{n,N} * \pi_{n,N} - \pi_{n,N}) (1 - \pi_{n,N}) + O(\epsilon^{N+2})
= \pi_{n,N} * (\pi_{n,N} * \pi_{n,N} - \pi_{n,N}) * (1 - \pi_{n,N}) + O(\epsilon^{N+2})
= (\pi_{n,N} * \pi_{n,N} - \pi_{n,N}) * \pi_{n,N} * (1 - \pi_{n,N}) + O(\epsilon^{N+2})
= -\epsilon^{2(N+1)} a_{n,N} * a_{n,N} + O(\epsilon^{N+2}) = O(\epsilon^{N+2})$$
(2.29)

where associativity of the Moyal product was used.

Accordingly, the off diagonal pieces of $\pi_n^{(N+1)}$ are still undetermined. We use the second condition in (2.19) to fix it. With the notation $[f,g]_*=f*g-g*f$ we have

$$[\pi_{n,N+1}, h]_{*} = [\pi_{n,N}, h]_{*} + \epsilon^{N+1} [\pi_{n}^{N+1}, h]_{*}$$

$$= [\pi_{n,N}, h]_{*} + \epsilon^{N+1} [\pi_{n}^{N+1}, h]_{*}$$

$$= \epsilon^{N+1} \{b_{n,N} + [\pi_{n}^{N+1}, \hat{h}_{0}]_{*}\} + O(\epsilon^{N+2})$$

$$= \epsilon^{N+1} \{b_{n,N} + [\pi_{n}^{N+1}, \hat{h}_{0}]\} + O(\epsilon^{N+2})$$
(2.30)

Accordingly

$$b_{n,N} + [\pi_n^{(N+1)}, \hat{h}_0] = 0 (2.31)$$

Projecting to the block diagonal pieces we obtain the consistency conditions using $[P_n, \hat{h}_0] = 0 = [P_n^{\perp}, \hat{h}_0]$

$$0 = P_n b_{n,N} P_n + [P_n \pi_n^{(N+1)} P_n, \hat{h}_0] = P_n b_{n,N} P_n - [P_n a_{n,N} P_n, \hat{h}_0]$$

$$0 = P_n^{\perp} b_{n,N} P_n^{\perp} + [P_n^{\perp} \pi_n^{(N+1)} P_n^{\perp}, \hat{h}_0] = P_n^{\perp} b_{n,N} P_n^{\perp} + [P_n^{\perp} a_{n,N} P_n^{\perp}, \hat{h}_0]$$

$$(2.32)$$

Indeed, again using the defining equations (2.22)

$$\{P_{n}b_{n,N}P_{n} - [P_{n}a_{n,N}P_{n},\hat{h}_{0}]\}\epsilon^{N+1} = \{P_{n}[\pi_{n,N},h]_{*}P_{n} - [P_{n}(\pi_{n,N}*\pi_{n,N}-\pi_{n,N})P_{n},\hat{h}_{0}]\} + O(\epsilon^{N+2})$$

$$= P_{n}\{[\pi_{n,N},h]_{*} - [(\pi_{n,N}*\pi_{n,N}-\pi_{n,N}),\hat{h}_{0}]_{*}\}P_{n} + O(\epsilon^{N+2})$$

$$= P_{n}\{[\pi_{n,N},h]_{*} - [(\pi_{n,N}*\pi_{n,N}-\pi_{n,N}),\hat{h}_{0}]_{*}\}P_{n} + O(\epsilon^{N+2})$$

$$= P_{n}\{[\pi_{n,N},h]_{*} - [(\pi_{n,N}*\pi_{n,N}-\pi_{n,N}),h]_{*}\}P_{n} + O(\epsilon^{N+2})$$

$$= P_{n}\{2[\pi_{n,N},h]_{*} - [\pi_{n,N}*\pi_{n,N},h]_{*}\}P_{n} + O(\epsilon^{N+2})$$

$$= P_{n}\{[(2\pi_{n,N}-\pi_{n,N}*\pi_{n,N}),h]_{*}\}P_{n} + O(\epsilon^{N+2})$$

$$= \pi_{n,N}*\{[(2\pi_{n,N}-\pi_{n,N}*\pi_{n,N}),h]_{*}\}*\pi_{n,N} + O(\epsilon^{N+2})$$

$$= 2\pi_{n,N}*[\pi_{n,N},h]_{*}*\pi_{n,N} - \pi_{n,N}*\pi_{n,N},h]_{*}*\pi_{n,N} - \pi_{n,N}*[\pi_{n,N},h]_{*}*\pi_{n,N} + O(\epsilon^{N+2})$$

$$= (\pi_{n,N}-\pi_{n,N})*[\pi_{n,N},h]_{*}*\pi_{n,N} + \pi_{n,N}*[\pi_{n,N},h]_{*}*(\pi_{n,N}-\pi_{n,N}*\pi_{n,N}) + O(\epsilon^{N+2})$$

$$= (\pi_{n,N}-\pi_{n,N})*[\pi_{n,N},h]_{*}*\pi_{n,N} + \pi_{n,N}*[\pi_{n,N},h]_{*}*(\pi_{n,N}-\pi_{n,N}*\pi_{n,N}) + O(\epsilon^{N+2})$$

$$= O(\epsilon^{N+2})$$

$$(2.33)$$

Similarly

$$\begin{aligned}
&\{P_{n}^{\perp}b_{n,N}P_{n}^{\perp} + [P_{n}^{\perp}a_{n,N}P_{n}^{\perp},\hat{h}_{0}]\}\epsilon^{N+1} = \{P_{n}^{\perp}[\pi_{n,N},h]_{*}P_{n}^{\perp} + [P_{n}^{\perp}(\pi_{n,N}*\pi_{n,N}-\pi_{n,N})P_{n}^{\perp},\hat{h}_{0}]\} + O(\epsilon^{N+2}) \\
&= P_{n}^{\perp}\{[\pi_{n,N},h]_{*} + [(\pi_{n,N}*\pi_{n,N}-\pi_{n,N}),\hat{h}_{0}]\}P_{n}^{\perp} + O(\epsilon^{N+2}) \\
&= P_{n}^{\perp}\{[\pi_{n,N},h]_{*} + [(\pi_{n,N}*\pi_{n,N}-\pi_{n,N}),\hat{h}_{0}]_{*}\}P_{n}^{\perp} + O(\epsilon^{N+2}) \\
&= P_{n}^{\perp}\{[\pi_{n,N},h]_{*} + [(\pi_{n,N}*\pi_{n,N}-\pi_{n,N}),h]_{*}\}P_{n}^{\perp} + O(\epsilon^{N+2}) \\
&= P_{n}^{\perp}[\pi_{n,N}*\pi_{n,N},h]_{*}\}P_{n}^{\perp} + O(\epsilon^{N+2}) \\
&= \pi_{n,N}^{\perp}*[\pi_{n,N}*\pi_{n,N},h]_{*}*\pi_{n,N} \perp + O(\epsilon^{N+2}) \\
&= \pi_{n,N}^{\perp}*\pi_{n,N}[\pi_{n,N},h]_{*}*\pi_{n,N}^{\perp} + \pi_{n,N}^{\perp}*[\pi_{n,N},h]_{*}*\pi_{n,N} + O(\epsilon^{N+2}) \\
&= O(\epsilon^{N+2})
\end{aligned} \tag{2.34}$$

Thus indeed (2.31) is only a condition on the block off diagonal projections

$$P_n b_{n,N} P_n^{\perp} + [P_n \pi_n^{(N+1)} P_n^{\perp}, \hat{h}_0] = 0 = P_n^{\perp} b_{n,N} P_n + [P_n^{\perp} \pi_n^{(N+1)} P_n, \hat{h}_0]$$
(2.35)

We only use the first condition of (2.35) as the second follows by taking the adjoint of the first if we manage to keep symmetry of $\pi_n^{(N+1)}$. We have with $f_{n,N+1}:=P_n\pi_n^{(N+1)}P_n^{\perp}$ using $P_n^2=P_n,\;[P_n,\hat{h}_0]=0$

$$[f_{n,N+1},\hat{h}_0] = f_{n,N+1}(P_n^{\perp}\hat{h}_0P_n^{\perp}) - (P_n\hat{h}_0P_n)f_{n,N+1} = f_{n,N+1}\left(\sum_{m\neq n}E_mP_m\right) - E_n\ c_{n,N+1}\ P_n^{\perp}$$

$$= f_{n,N+1}(\sum_{m \neq n} (E_m - E_n) P_m) =: f_{n,N+1} \hat{h}_{0n}^{\perp}$$
(2.36)

The operator \hat{h}_{0n}^{\perp} has the inverse on $P_n^{\perp}\mathcal{H}_f$ given by

$$\Delta_n := \sum_{m \neq n} (E_m - E_n)^{-1} P_m \tag{2.37}$$

provided the no band crossing condition $E_m(z) - E_n(z) \neq 0$ for all $z, m \neq n$ holds. As mentioned before the strongest condition would be that gap number

$$g_n := \sup_{z,m \neq n} |E_m(z) - E_n(z)|$$
 (2.38)

should be positive but we will not rely on this in our purely formal investigation. Thus we find

$$f_{n,N+1} = -P_n b_{n,N} P_n^{\perp} \Delta_n \tag{2.39}$$

Note that both the l.h.s. and the r.h.s. of (2.39) annihilate $P_n\mathcal{H}_f$.

Collecting all terms we thus have computed

$$\pi_n^{(N+1)} = -P_n a_{n,N} P_n + P_n^{\perp} a_{n,N} P_n^{\perp} - P_n b_{n,N} P_n^{\perp} \Delta_n + \Delta_n P_n^{\perp} b_{n,N} P_n \tag{2.40}$$

from $a_{n,N}$, $b_{n,N}$ given in (2.22). One easily checks that (2.40) is symmetric.

2.2.2 Construction of the Moyal unitarities

We now turn to constructing $u_{n,N+1}$ from $u_{n,N},\pi_{n,N+1}$. We isolate the leading orders

$$u_{n,N} * u_{n,N}^{\dagger} - 1_f =: \epsilon^{N+1} c_{n,N} + O(\epsilon^{N+2}), \ u_{n,N}^{\dagger} * u_{n,N} - 1_f =: \epsilon^{N+1} e_{n,N} + O(\epsilon^{N+2}),$$

$$u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} - r_n =: \epsilon^{N+1} d_{n,N} + O(\epsilon^{N+2})$$
(2.41)

with $c_{n,N}, d_{n,N}, e_{n,N}$ symmetric and find

$$u_{n,N+1} * u_{n,N+1}^{\dagger} - 1_{f} = [u_{n,N} * u_{n,N}^{\dagger} - 1_{f}] + \epsilon^{N+1} \{ u_{n}^{(N+1)} * u_{n,N}^{\dagger} + u_{n,N} * (u_{n}^{(N+1)})^{\dagger} \}$$

$$+ \epsilon^{2(N+1)} u_{n}^{(N+1)} * (u_{n}^{(N+1)})^{\dagger}$$

$$= \{ c_{n,N} + u_{n}^{(N+1)} * u_{n,0}^{\dagger} + u_{n,0} * (u_{n}^{(N+1)})^{\dagger} \} \epsilon^{N+1} + O(\epsilon^{N+2})$$

$$= \{ c_{n,N} + u_{n}^{(N+1)} u_{n,0}^{\dagger} + u_{n,0} (u_{n}^{(N+1)})^{\dagger} \} \epsilon^{N+1} + O(\epsilon^{N+2})$$

$$(2.42)$$

Similarly

$$u_{n,N+1}^{\dagger} * u_{n,N+1} - 1_f = \{e_{n,N} + (u_n^{(N+1)})^{\dagger} u_{n,0} + u_{n,0}^{\dagger} u_n^{(N+1)}\} \epsilon^{N+1} + O(\epsilon^{N+2})$$
(2.43)

and

$$u_{n,N+1} * \pi_{n,N+1} * u_{n,N+1}^{\dagger} - r_n = \epsilon^{N+1} \{ d_{n,N} + u_{n,0} \pi_n^{(N+1)} u_{n,0}^{\dagger} + u_n^{(N+1)} \pi_{n,0} u_{n,0}^{\dagger} u_{n,0} \pi_{n,0} (u_n^{(N+1)})^{\dagger} \} + O(\epsilon^{N+2})$$
(2.44)

Accordingly

$$0 = c_{n,N} + u_n^{(N+1)} u_{n,0}^{\dagger} + u_{n,0} (u_n^{(N+1)})^{\dagger}$$

$$0 = e_{n,N} + (u_n^{(N+1)})^{\dagger} u_{n,0} + u_{n,0}^{\dagger} u_n^{(N+1)}$$

$$0 = d_{n,N} + u_{n,0} \pi_n^{(N+1)} u_{n,0}^{\dagger} + u_n^{(N+1)} \pi_{n,0} u_{n,0}^{\dagger} u_{n,0} \pi_{n,0} (u_n^{(N+1)} 2.45)^{\dagger}$$

We isolate $(u_n^{(N+1)})^{\dagger}$ from the first two equations

$$(u_n^{(N+1)})^{\dagger} = -u_{n,0}^{\dagger}(c_{n,N} + u_n^{(N+1)}u_{n,0}^{\dagger}) = -(e_{n,N} + u_{n,0}^{\dagger}u_n^{(N+1)})u_{n,0}^{\dagger}$$
(2.46)

implying the identity

$$e_{n,N}u_{n,0}^{\dagger} - u_{n,0}^{\dagger}c_{n,N} = 0 (2.47)$$

This is identically satisfied by induction assumption since

$$(e_{n,N}u_{n,0}^{\dagger} - u_{n,0}^{\dagger}c_{n,N})\epsilon^{N+1} = (u_{n,N}^{\dagger} * u_{n,N} - 1_f)u_{n,0}^{\dagger} - u_{n,0}^{\dagger}(u_{n,N} * u_{n,N}^{\dagger} - 1_f) + O(\epsilon^{N+2})$$

$$= (u_{n,N}^{\dagger} * u_{n,N} - 1_f) * u_{n,0}^{\dagger} - u_{n,0}^{\dagger} * (u_{n,N} * u_{n,N}^{\dagger} - 1_f) + O(\epsilon^{N+2})$$

$$= (u_{n,N}^{\dagger} * u_{n,N} - 1_f) * u_{n,N}^{\dagger} - u_{n,N}^{\dagger} * (u_{n,N} * u_{n,N}^{\dagger} - 1_f) + O(\epsilon^{N+2})$$

$$= O(\epsilon^{N+2})$$
(2.48)

Accordingly we may use henceforth

$$e_{n,N} = u_{n,0}^{\dagger} c_{n,N} u_{n,0}^{\dagger} \tag{2.49}$$

Substituting (2.46) into the third relation of (2.45) yields

$$-(d_{n,N} + u_{n,0}\pi_n^{(N+1)}u_{n,0}^{\dagger}) = u_n^{(N+1)}\pi_{n,0}u_{n,0}^{\dagger} - u_{n,0}\pi_{n,0}u_{n,0}^{\dagger}(c_{n,N} + u_n^{(N+1)}u_{n,0}^{\dagger})$$

$$= u_n^{(N+1)}u_{n,0}^{\dagger}r_n - r_n(c_{n,N} + u_n^{(N+1)}u_{n,0}^{\dagger})$$

$$= -r_nc_{n,N} + [u_n^{(N+1)}u_{n,0}^{\dagger}, r_n]$$
(2.50)

or

$$[r_n, u_n^{(N+1)} u_{n,0}^{\dagger}] = d_{n,N} + u_{n,0} \pi_n^{(N+1)} u_{n,0}^{\dagger} - r_n c_{n,N}$$
(2.51)

Projecting with r_n or $r_n^{\perp}=1_f-r_n$ from both sides gives the identities

$$0 = r_n(d_{n,N} + u_{n,0}\pi_n^{(N+1)}u_{n,0}^{\dagger} - r_n c_{n,N})r_n = r_n^{\perp}(d_{n,N} + u_{n,0}\pi_n^{(N+1)}u_{n,0}^{\dagger} - r_n c_{n,N})r_n^{\perp}$$
(2.52)

which are again identically satisfied by induction assumption since, remembering (2.40) which we write in the form (and using $P_n^{\perp}\Delta_n=\Delta_nP_n^{\perp}=\Delta_n$)

$$u_{n,0}\pi_{n}^{(N+1)}u_{n,0}^{\dagger} = -r_{n}u_{n,0}a_{n,N}u_{n,0}^{\dagger}r_{n} + r_{n}^{\perp}u_{n,0}a_{n,N}u_{n,0}^{\dagger}r_{n}^{\perp} - r_{n}u_{n,0}b_{n,N}\Delta_{n}u_{n,0}^{\dagger}r_{n}^{\perp} + r_{n}^{\perp}u_{n,0}\Delta_{n}b_{n,N}u_{n,0}^{\dagger}r_{n} - r_{n}u_{n,0}b_{n,N}\Delta_{n}u_{n,0}^{\dagger}r_{n}^{\perp} + r_{n}^{\perp}u_{n,0}\Delta_{n}b_{n,N}u_{n,0}^{\dagger}r_{n}^{\perp} + r_{n}^{\perp}u_{n,0}\Delta_{n}b_{n,N}u_{n,0}^{\perp}r_{n}^{\perp} + r_{n}^{\perp}u_{n,0}\Delta_{n}b_{n,N}u_{n,0}^{\perp}r_{n}^{\perp} + r_{n}^{\perp}u_{n,0}\Delta_{n}b_{n,N}u_{n,0}^{\perp}r_{n}^{\perp} + r_{n$$

whence

$$\epsilon^{N+1} r_{n} (d_{n,N} + u_{n,0} \pi_{n}^{(N+1)} u_{n,0}^{\dagger} - r_{n} c_{n,N}) r_{n} = \epsilon^{N+1} r_{n} (d_{n,N} - u_{n,0} a_{n,N} u_{n,0}^{\dagger} - c_{n,N}) r_{n}$$

$$= r_{n} ([u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} - r_{n}] - u_{n,0} [\pi_{n,N} * \pi_{n,N} - \pi_{n,N}] u_{n,0}^{\dagger} - [u_{n,N} * u_{n,N}^{\dagger} - 1_{f}]) r_{n} + O(\epsilon^{N+2})$$

$$= r_{n} (u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} - u_{n,0} * (\pi_{n,N} * \pi_{n,N} - \pi_{n,N}) * u_{n,0}^{\dagger} - u_{n,N} * u_{n,N}^{\dagger}) r_{n} + O(\epsilon^{N+2})$$

$$= r_{n} u_{n,N} * (\pi_{n,N} - \pi_{n,N} * \pi_{n,N} + \pi_{n,N} - 1_{f}) * u_{n,N}^{\dagger} r_{n} + O(\epsilon^{N+2})$$

$$= -r_{n} u_{n,N} * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * u_{n,N}^{\dagger} r_{n} + O(\epsilon^{N+2})$$

$$(2.54)$$

We abbreviate the following $O(\epsilon^{N+1})$ objects

$$D_n := u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} - r_n, \ C_n := u_{n,N} * u_{n,N}^{\dagger} - 1_f, \ E_n := u_{n,N}^{\dagger} * u_{n,N} - 1_f, \ A_n := \pi_{n,N} * \pi_{n,N} - \pi_{n,N}$$

$$(2.55)$$

any bilinear combination of which is thus of order ϵ^{N+2} and continue (2.54) (in the first step, use that r_n is a constant on the slow phase space)

$$r_{n}u_{n,N} * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * u_{n,N}^{\dagger} r_{n} + O(\epsilon^{N+2})$$

$$= r_{n} * u_{n,N} * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * u_{n,N}^{\dagger} * r_{n} + O(\epsilon^{N+2})$$

$$= (u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} - D_{n}) * u_{n,N} * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * u_{n,N}^{\dagger} * (u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} - D_{n}) + O(\epsilon^{N+2})$$

$$= u_{n,N} * \pi_{n,N} * (u_{n,N}^{\dagger} * u_{n,N}) * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * (u_{n,N}^{\dagger} * u_{n,N}) * \pi_{n,N} * u_{n,N}^{\dagger}$$

$$- D_{n} * u_{n,N} * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * (u_{n,N}^{\dagger} * (u_{n,N}) * \pi_{n,N} * u_{n,N}^{\dagger})$$

$$- D_{n} * u_{n,N} * (u_{n,N}^{\dagger} * u_{n,N}) * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * u_{n,N}^{\dagger} * (u_{n,N} * \pi_{n,N} * D_{n} + O(\epsilon^{N+2})$$

$$= u_{n,N} * \pi_{n,N} * (E_{n} + 1_{f}) * (\pi_{n,N} - 1_{f}) * (E_{n} + 1_{f}) * \pi_{n,N} * u_{n,N}^{\dagger}$$

$$- D_{n} * u_{n,N} * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * (E_{n} + 1_{f}) * \pi_{n,N} * u_{n,N}^{\dagger}$$

$$= -u_{n,N} * \pi_{n,N} * (E_{n} + 1_{f}) * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * u_{n,N}^{\dagger} * (u_{n,N} * \pi_{n,N} * D_{n} + O(\epsilon^{N+2})$$

$$= u_{n,N} * \pi_{n,N} * (E_{n} + 1_{f}) * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * u_{n,N}^{\dagger} * (u_{n,N} * \pi_{n,N} * D_{n} + O(\epsilon^{N+2})$$

$$= u_{n,N} * \pi_{n,N} * (E_{n} + 1_{f}) * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * (\pi_{n,N} - 1_{f}) * (E_{n} + 1_{f}) * (E_{n$$

The second identity in (2.52) follows similarly

$$\epsilon^{N+1} r_n^{\perp} (d_{n,N} + u_{n,0} \pi_n^{(N+1)} u_{n,0}^{\dagger} - r_n c_{n,N}) r_n^{\perp} = \epsilon^{N+1} r_n^{\perp} (d_{n,N} + u_{n,0} a_{n,N} u_{n,0}^{\dagger}) r_n^{\perp}$$

$$= r_n^{\perp} (u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} - r_n + u_{n,0} (\pi_{n,N} * \pi_{n,N} - \pi_{n,N}) u_{n,0}^{\dagger}) r_n^{\perp} + O(\epsilon^{N+2})$$

$$= r_n^{\perp} (u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} + u_{n,0} * (\pi_{n,N} * \pi_{n,N} - \pi_{n,N}) * u_{n,0}^{\dagger}) r_n^{\perp} + O(\epsilon^{N+2})$$

$$= r_n^{\perp} u_{n,N} * (\pi_{n,N} * + \pi_{n,N} * \pi_{n,N} - \pi_{n,N}) * u_{n,N}^{\dagger} r_n^{\perp} + O(\epsilon^{N+2})$$

$$= r_n^{\perp} * u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} * r_n^{\perp} + O(\epsilon^{N+2})$$

$$= (1_f - u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} - D_n) * u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} * (1_f - u_{n,N} * \pi_{n,N} * u_{n,N}^{\dagger} - D_n) + O(\epsilon^{N+2})$$

$$= (u_{n,N} * (1_f - \pi_{n,N} * u_{n,N}^{\dagger} * u_{n,N}) - D_n * u_{n,N}) * \pi_{n,N} * \pi_{n,N} * (1_f - u_{n,N}^{\dagger} * u_{n,N} * u_{n,N}^{\dagger}) + O(\epsilon^{N+2})$$

$$= (u_{n,N} * (1_f - \pi_{n,N} * u_{n,N}^{\dagger} * u_{n,N}) * u_{n,N}^{\dagger} - u_{n,N}^{\dagger} * D_n) + O(\epsilon^{N+2})$$

$$= (u_{n,N} * (1_f - \pi_{n,N} * (1_f + E_n)) - D_n * u_{n,N}) * \pi_{n,N} * \pi_{n,N} * (1_f - (1_f + E_n) * \pi_{n,N}) * u_{n,N}^{\dagger} - u_{n,N}^{\dagger} * D_n) + O(\epsilon^{N+2})$$

$$= [u_{n,N} * A_n - (u_{n,N} * \pi_{n,N} * E_n + D_n * u_{n,N}) * \pi_{n,N}] * \pi_{n,N} * (A_n * u_{n,N}^{\dagger} - \pi_{n,N} * (E_n * u_{n,N}^{\dagger} + u_{n,N}^{\dagger} * D_n) + O(\epsilon^{N+2})$$

$$= O(\epsilon^{N+2})$$

where we again used constancy of r_n .

It follows that the block diagonal pieces of $u_n^{(N+1)}$ wrt r_n remain undetermined (we can choose them to vanish for simplicity). We thus project to the block off diagonal parts of (2.51) using again

(2.53)

$$r_{n}u_{n}^{(N+1)}u_{n,0}^{\dagger}r_{n}^{\perp} = r_{n}(d_{n,N} + u_{n,0}\pi_{n}^{(N+1)}u_{n,0}^{\dagger} - r_{n}c_{n,N})r_{n}^{\perp}$$

$$= r_{n}(d_{n,N} - u_{n,0}b_{n,N}\Delta_{n}u_{n,0}^{\dagger} - c_{n,N})r_{n}^{\perp}$$

$$-r_{n}^{\perp}u_{n}^{(N+1)}u_{n,0}^{\dagger}r_{n} = r_{n}^{\perp}(d_{n,N} + u_{n,0}\pi_{n}^{(N+1)}u_{n,0}^{\dagger} - r_{n}c_{n,N})r_{n}$$

$$= r_{n}^{\perp}(d_{n,N} + u_{n,0}\Delta_{n}b_{n,N}u_{n,0}^{\dagger})r_{n}$$
(2.58)

Accordingly, if we indeed assume the block off diagonal terms to vanish for simplicity since $u_{n,N}$ is just an auxiliary structure we find explicitly

$$u_n^{(N+1)} = \{ r_n (d_{n,N} - u_{n,0} b_{n,N} \Delta_n u_{n,0}^{\dagger} - c_{n,N}) r_n^{\perp} - r_n^{\perp} (d_{n,N} + u_{n,0} \Delta_n b_{n,N} u_{n,0}^{\dagger}) r_n \} u_{n,0}$$
(2.59)

2.2.3 Effective Hamiltonian

This concludes the perturbative construction. Using equations (2.22), (2.40), (2.41), (2.49) and (2.59) we can compute $\pi_{n,N}$, $u_{n,N}$ up to any finite order N. As outlined in section 2.1 we now construct the *effective symbol*

$$h_{n,N} = r_n (u_{n,N} * h * u_{n,N}^{\dagger}) r_n \tag{2.60}$$

and from this the effective Hamiltonian

$$H_{n,N} = W(h_{n,N}) = R_n U_{n,N} H U_{n,N}^{\dagger} R_n$$
 (2.61)

that preserves the subspace $R_n\mathcal{H}$. That subspace carries the orthonormal basis $b_{n,a}\otimes s_\alpha,\ a=1,..,d_n$ and s_α denotes an ONB of \mathcal{H}_s . The spectrum $E_{n,N}$ of $H_{n,N}$ gives an approximation of order ϵ^{N+1} of the n-th energy band E_n of H. The advantage of $H_{N,n}$ is that it is effectively an operator on the rather small Hilbert space $\mathbb{C}^{d_n}\otimes\mathcal{H}_s$ while backreaction effects between the slow and fast sector are taken care of to the given order of approximation.

3 Challenges of cosmological SAPT

As mentioned in the introduction and as it also transpires from the previous section, SAPT was designed for quantum theories with a finite number of degrees of freedom. When we try to generalise to quantum field theories such as second order quantum cosmological perturbation theory, we meet challenges because some of the assumptions of the quantum mechanical setting do not automatically transfer to the QFT case. Here the role of the fast degrees of freedom is played by the infinite number of inhomogeneous perturbations while the slow ones are the homogeneous modes. We will show this below, for the time being it may be sufficient to say that when cutting off the number of inhomogeneous modes in an intermediate step in order to be in the quantum mechanical setting of SAPT we can consider the system as a "gas" with a finite number of particles and the homogeneous mode takes the role of the centre of mass degree of freedom. Note that the volume of the "gas" is finite because our models, even when considering only the classical level, are only well defined when the spatial slices are compact.

As we will see, these kind of problems originating from the infinite number of degrees of freedom can be circumvented using a canonical transformation of the total system involving both homogeneous and inhomogeneous modes which is exact up top second order in the perturbations. Here we will borrow ideas developed for the hybrid approach to Lopp Quantum Cosmology (LQC) [9]. However, then one meets the next problem: The mass squared functions that enter the quantum field perturbation get modified as a result of that canonical transformation and are generically neither positive definite nor are they polynomials in the slow (homogeneous) degrees of freedom, an example

being the Mukhanov-Sasaki mass squared term. The latter property is already met for the purely homogeneous contribution to the Hamiltonian constraint, however, the degree of npn-polynomiality gets *much worsened*. As there is some amount of freedom in the choice of that canonical transformation, the indefiniteness of the mass squared term could perhaps be avoided by exploiting that freedom, however at the present stage of research we are not sure that this is the case and thus prepare ourselves for the worst case scenario.

As far as the first problem is concerned, we offer two kinds of solutions: Either one considers a further canonical transformation just of the slow sector to new variables in terms of which the masses are manifestly non negative and declares the phase space as defined in terms of the old variables to be restricted by the positivity of the masses. Or one has to switch off modes by hand for which the frequency becomes negative as suggested first in [18]. The first solution has the advantage that one stays within the standard QFT framework of positive mass squared, however at the price of making the Hamiltonian even less polynomial and by a possibly non-physical restriction of the phase space. The second solution has the advantage of not worsening the amount of non polynomiality and of not modifying the phase space of the slow sector, however, the physical interpretation of the mode off switching remains obscure: Typically this happens at the classical big bang singularity and in the limit of vanishing scale factor, all modes would need to be removed. One could speculate whether this presents a self-regulating effect of a new kind in the sense that the matter density and thus curvature automatically vanishes as we approach the singularity, thus eventually avoiding the big bang.

As far as the second problem is concerned, in LQC methods for dealing with non-polynomial expressions in momentum variables but polynomial in configuration variables adapted from techniques developed for the full theory [19] have been employed. These become available because one uses a representation of the slow sector of the theory which is not unitarily equivalent to the Schrödinger representation but only if one substitutes the unbounded configuration variable by a bounded polynomial of Weyl operators [10]. This latter step is motivated by the full theory where it appears in a regularisation procedure and in the limit of vanishing regulator the original polynomial is recovered. This regulator is of point splitting type (technically, it involves the coordinate area enclosed by a loop that labels a Wilson loop variable) and can be arbitrarily small in the full theory but not in LQC and thus stays there as a remnant that defines the model. Both in LQC and in full LQG what survives the limit of taking the regulator away is the substituting polynomial of Weyl operators that one put in. The possible effects of this kind of ambiguity have been recently pointed at for LQC in [20]. In LQG they have been much debated since their first occurence and there are several approaches to fix them. One of them [21, 22] is in the context of Dirac quantisation of the constraints and uses the representation theory of the hypersurface deformation algebra. Another one [23] exploits the possibility of gauge fixing before quantisation and applies standard Wilson type renormalisation to dynamical systems with a physical Hamiltonian (not constrained to vanish) [24]. However, a simple inspection of the Mukhanov-Sasaki mass squared term reveals that the techniques of [10] for the purely homogeneous contribution to the Hamiltonian constraint and of [9] for hybrid LQC will no longer be sufficient when backreaction is switched on. This is due to the fact that the adiabatic corrections introduce non polynomial functions of both momentum and configuration variables, in particular, negative powers of both variables occur.

We solve this second problem by taking an unbiased point of view towards quantisation of the homogeneous sector and try to stay within the standard Schrödinger representation as suggested by the Weyl quantisation method that enters the SAPT formalism. In the best case one should find a dense and invariant domain for the various non polynomial operators that appear. This is indeed possible for the model that also involves Gaussian dust by exploiting the existence of a remarkable basis of functions in $L_2(\mathbb{R}, dx)$ which is smooth and of rapid decrease both at infinity and at the origin [25]. For the case of the Mukhanov-Sasaki field we have to content ourselves by providing a dense but not invariant domain.

This section is organised as follows:

In the first subsection we explain in more detail why we can consider the homogeneous degrees of freedom as the slow sector of cosmological perturbation theory.

In the second we display the afore mentioned obstacle to SAPT in the QFT context and show how to solve it up to second order in the inhomogeneous perturbations. A key role is played here by a certain Hilbert-Schmidt condition.

In the third we describe the induced non positive, non-polynomial mass squared problem and apply both solution techniques sketched above based on either modifying the classical slow phase space or the number of physical modes in the Fock space.

In the fourth subsection we sketch a proposal for how to deal with the resulting highly non polynomial operators that occur as a result of the canonical transformations and the adiabatic corrections due to Moyal product.

3.1 Homogeneous sector as center of mass degrees of freedom

In our publications we are considering 4 different models:

- I. Coupled (an)harmonic oscillators
- II. Homogeneous isotropic GR coupled to homogeneous mode of the inflaton
- III. Homogeneous isotropic GR couupled to all modes of the inflaton in the presence of 4 deparametrising dust fields
- IV. GR coupled to an inflaton without deparametrising matter fields

Models I. and III. are unconstrained systems and the corresponding Hamiltonian is a physical Hamiltonian, in particular, it does not need to vanish, we are interested in the full spectrum and not only its kernel and we must not multiply the Hamiltonian with anything. Model IV. is a constrained system, we are only interested in the kernel of the Hamiltonian constraint and we are allowed to multiply the Hamiltonian with convenient (non-vanishing) factors if necessary. Model II. can be considered as the truncation of both model III and model IV. to the entirely homogeneous degrees of freedom. Thus it makes sense to consider the full spectrum of the corresponding Hamiltonian in model II.

When treating these models with SAPT techniques we notice that what makes SAPT work at the technical level is that one multiplies the momenta p of the "slow" degrees of freedom (q,p) with a small factor ϵ thus changing the canonical bracket $\{p,q\}=1$ into $\{p',q\}=\epsilon$ with $p'=\epsilon$. The factor ϵ is usually physically motivated by a corresponding parameter appearing in the Hamiltonian such as a ratio between small and large masses $\epsilon^2=m/M$. In the corresponding Moyal products of the corresponding Weyl quantisation the parameter ϵ then organises the perturbative expansion of the SAPT scheme. In order that this works, the corresponding Hamiltonian, when expressed in terms of the primed slow momenta, must not contain negative powers of ϵ . Interestingly, when the Hamiltonian is a constraint, then we can in fact always achieve that no negative powers appear by multiplying the constraint by sufficiently large powers of ϵ . We will exploit that freedom when treating model IV (and, when considered as a truncation of model IV, also model II).

For model I. the parameter ϵ^2 indeed has the interpretation of a mass ratio m/M. We notice that the physical intuition here is the equipartition theorem which states that in thermodynamical equilibrium at any non vanishing temeperature T the phase space average (and therefore the statistical = time average if the system is ergodic) of both p^2/M and $y^2//m$ is equal. Since $v=p/m,\ u=y/m$ (with (x,y) the fast d.o.f.) are the corresponding velocities we find $v=\epsilon u\ll u$. Note that this has nothing to do with the frequencies of the oscillators. Even if the frequency Ω of the heavy oscillator is much larger than that ω of the fast oscilltor we still have $v\ll u$. This is possible because $v=b\Omega, u=a\omega$ for amplitudes b,a and we then have $b/a\ll \epsilon$.

For model II. we interpret $\epsilon^2=\kappa/\lambda=:m/M$ where λ,κ are the inflaton and gravitational coupling constants. Note that $\hbar\kappa$ is the Planck area and $\hbar\lambda$ also has the dimension of an area. Note also that λ is to be distinguished from the Compton wave length $l=\hbar/(\mu c)$ where μ is the Klein Gordon mass (i.e. $2\mu=V''(\phi=0)$ for the potential V of the inflaton ϕ). In the SAPT treatment

we will assume that $\kappa/\lambda \ll 1$ which would be the case if $\hbar\lambda \approx l^2$ which one assumes to be of the order of length scale of the standard model. The equipartition theorem does not work for this model because in deriving

$$< p^2/M > = < y^2/m >, < f > := \frac{\int dq \, dp \, dx \, dy \, e^{-\beta H} \, f}{\int dq \, dp \, dx \, dy \, e^{-\beta H} \, 1}$$
 (3.1)

one assumes that H is bounded from below so that the integrals converge and that in the integrations by parts that one performs to show that $< p(\partial H/\partial p) >= \beta^{-1}$ no boundary terms appear. Both conditions are violated in model II because the gravitational kinetic energy is negative. However we use the fact that the Hamiltonian is a constraint. Therefore up to numerical constants

$$p^{2}/(Ma) = M\Lambda a^{3} + \pi_{0}^{2}/(ma^{3}) + ma^{3}V(\phi_{0})$$
(3.2)

with p,π_0 the homogeneous momenta of scale factor and inflaton respectively. Since $v=\ln(a)=-p/(Ma^2),~\dot{\phi}=u=\pi/(ma^3)$ we find

$$Mv^2 = [M\Lambda + m(u^2 + V)] \tag{3.3}$$

displaying again $v \ll u$ for very small Λ and potential at least. Accordingly, the zero (homogenous) mode of the inflaton is "fast" while homogeneous gravity mode is "slow" owing to our assumption on λ, κ .

Model III. exhibits new challenges due to the inhomogeneous modes of the inflaton. Note however, that the inflaton here is a gauge invariant degree of freedom because the constraints have already been solved using reduced phase space methods. In particular, there is no motivation from the gauge perspective to split the inflaton into zero mode (homogenous part) and the rest as it is the case for the hybrid treatment of model IV. There are no linearised constraints etc. In order to meet the Hilbert Schmidt condition (simultaneous existence of a Fock representation supportying the Hamiltonian and a representation of the gravitational d.o.f.), after a canonical transformation exact up to second order the Klein Gordon mass m^2 gets modified into μ^2 and displays a phase space dependence with respect to the homogeneous gravitational d.o.f. but not the zero mode of the inflaton, it does not depend on the inflaton d.o.f. at all. That mass dependence is such that p only appears in the combination $p^2\kappa^2=\epsilon^4\lambda^2p^2=\epsilon^2\lambda^2(p')^2$. i.e. only positive powers of ϵ appear in μ^2 when expressed in terms of p'. Since the Hamiltonian is still not bounded from below, the equipartition theorem can again not be used to argue that the (p, a) are slow compared to all inflaton modes. However, the physical Hamiltonian H results from a constraint of the form C = P + H = 0 where P is the energy density of the dust. As the dust behaves closely to a field of test observers with zero energy density, P is very small and thus H is close to zero. Thus we can argue and apply the SAPT scheme as for model II if we assume that all inflaton modes are at least as fast as its homogeneous ones. See below for a

Finally in model IV. we treat both the gravitational tensor modes (graviton) and the gauge invariant extension of the inflaton (Mukhanov-Sasaki (MS) field ν) using the hybrid scheme (the vector modes are not gauge invariant to first odrder and are dropped). Due to the requirement of linearised gauge invariance, the mass squared term μ^2 of ν as well as the mass squared term ρ^2 of the graviton acquire a phase space dependence wrt both the homogneous inflaton as well as homogenous gravitational dof. Additional phase space dependence of μ^2 , ρ^2 with respect to these d.o.f. is generated by a HS condition guaranteeing canonical transformation as for model III. Due to the additional dependence of μ^2 , ρ^2 on the homogeneous inflaton d.o.f. (π_0, ϕ_0) it is necessary to show that these also "slow" as compared to the inhomogeneous d.o.f. (ν, π_{ν}) and (h^{ab}, π_{ab}) if we want to use the SAPT scheme. The graviton piece of the Hamiltonian reads (up to powers of a)

$$\kappa \pi^{ab} \pi_{ab} + h^{ab} (-\Delta/\kappa + \rho^2) h_{ab} \tag{3.4}$$

To make it look like the MS piece

$$\lambda \pi_{\nu}^2 + \nu (-\Delta/\lambda + \mu^2)\nu \tag{3.5}$$

we perform the canonical transformation $\tilde{\pi}^{ab} = \epsilon \pi^{ab}$, $\tilde{h}_{ab} = \epsilon^{-1} h_{ab}$ so that (3.4) becomes

$$\lambda \tilde{\pi}^{ab} \tilde{\pi}_{ab} + \tilde{h}^{ab} (-\Delta/\lambda + \tilde{\rho}^2) \tilde{h}_{ab} \tag{3.6}$$

where $\tilde{\rho}^2=\epsilon^2\rho^2$. An explicit check reveals that both the MS mass μ^2 as well as $\tilde{\rho}^2$ receive only non negative powers of ϵ when expressed in terms of

$$\tilde{p} = \epsilon^2 p = \epsilon p', \ \tilde{\pi_0} = \epsilon \pi_0$$
 (3.7)

Note that while in model II we used $p', \pi'_0 = \pi_0$ instead of $\tilde{p}, \tilde{\pi}$ we still have $\tilde{p}/\tilde{\pi} = p'/\pi'$. This corresponds to the fact that when multiplying model II viewed as the homogenous truncation of model IV by ϵ^2 we could have as well worked with $\tilde{p}, \tilde{\pi}$.

The only problem is that the homogeneous piece of the Hamiltonian constraint of model IV cannot be written in terms of $\tilde{p}, \tilde{\pi}$ without picking up negative powers of ϵ . But this can be repaired, as remarked above and following the observation just made by multiplying the *entire* constraint including the inhomogeneous MS and graviton pieces by ϵ^2 . We now perform again a canonical transformation $\hat{\pi}_{\nu}=\epsilon\pi_{\nu},~\hat{\nu}=nu/\epsilon$ and similar for the graviton variables to write the constraint in terms of

$$\lambda \hat{\pi}_{\nu}^{2} + \hat{\nu} \epsilon^{4} (-\Delta/\lambda + \mu^{2}) \hat{\nu} \tag{3.8}$$

and similar for the graviton piece. Defining $\omega^2=-\Delta/\lambda+\mu^2$ we now define the Fock representation by the annihilation operator

$$\hat{b} = \left[\epsilon\sqrt{\omega}\hat{\nu} - i(\epsilon\sqrt{\omega})^{-1}\hat{\pi}_{\nu}\right]/\sqrt{2}$$
(3.9)

Remarkably $\tilde{b}=b$ is exactly the same annihilation operator as one would have defined before that last canonical transformation (i.e. resubstituting ν,π_{ν}), i.e. the Fock representations are identical. When normal ordered one finds that the MS Hamiltonian becomes

$$\epsilon^2 \int d^3x \ b^{\dagger} \omega^2 b \tag{3.10}$$

ie. the spectrum of the inhomogeneous part of the constraint gets simply rescaled by ϵ^2 and one can use all the results of the original Fock representation. This is in fact neat as one would expect that the homogeneous modes alone as corresponding to model II multiplied by ϵ^2 are little disturbed by the inhomogeneous ones.

In summary, all one has to do is a simple rescaling $p \to \epsilon^2 p = \tilde{p}, \ \pi \to \epsilon \pi - \tilde{\pi}$ in order to use the SAPT scheme in model IV and this is consistent with the treatment of model II.

In fact, we can also treat model III consistently this way by simply multiplying (and, to get the correct spectrum, afterwards dividing) by ϵ^2 thus working in all models II., III. and IV. consistently with $\tilde{p}, \tilde{\pi}$.

What is missing is the justification for why the homogeneous scalar field mode should be slower than the inhomogeneous modes in model IV and for completeness also in model III although there it would be sufficient that all inflaton modes are equally fast. It turns out that the answer to the question lies in the definition of the modes. By homogeneous mode we losely speaking mean a component of the field which does not depend on position. But this becomes unambiguous only when relating it to the full field. Given the torus of volume L^3 we consider the mode system e_I , $I \in \mathbb{Z}^3$, $e_I(x) = \exp(ik_L I \cdot x)$, $k_L = 2\pi/L$ which enjoy

$$\langle e_I, e_J \rangle = L^3 \delta_{I,J}, \ \frac{1}{L^3} \sum_n e_I \langle e_I, . \rangle = 1_{L_2}, \langle f, g \rangle = \int_{[0,L]^3} d^3x \ f^*(x) \ g(x)$$
 (3.11)

periodic boundary conditions understood. We define the homogenous modes of say a scalar field ϕ,π by

$$\overline{\phi} := \frac{1}{L^3} \int d^3x \, \phi(x) = \langle e_0, \phi \rangle / L^3, \ \overline{\pi} := \frac{1}{L^3} \int d^3x \, \pi(x) = \langle e_0, \pi \rangle / L^3$$
 (3.12)

which are easily checked to have canonical brackets $\{\overline{\pi},\overline{\phi}\}=\frac{1}{L^3}$ if $\{\pi(x),\phi(y)\}=\delta(x,y)$. We see already that the local point modes $\phi(x),\pi(x)$ are "infinitely faster" than the homogenous modes because $\delta(x,x)=\infty$. To understand this in more detail we note that SAPT was developed for quantum mechanical systems with a finite number of degrees of freedom. Accordingly we regularise the Hamiltonian using a finite resolution cut-off $\delta_N=L/N$ and a finite number of position localised degrees of freedom $\phi_I^N=\int d^3x~\chi_{N,I}(x)~\phi(x)/delta_N^3$ and similar for π_n^N where $\chi_{N,I}$, $I\in\mathbb{N}_N^3$, $\mathbb{N}_N=\{0,1,2,..,N-1\}$ is a partition of the torus into disjoint cubes of volume δ_N^3 . We check that $\{\pi_I^N,\phi_J^N\}=\delta_{I,J}/\delta_N^3$ so that $\overline{\phi}$ is slower than any of the ϕ_I^N by a factor of N^3 . In fact we note the identity $\overline{\phi}=\frac{1}{N^3}\sum_{I\in\mathbb{N}_N^3}\phi_I^N$. We see that $\overline{\phi}$ is the *centre of mass coordinate* of a system of N^3 coordinates ϕ_I^N of equal mass. Thus at finite resolution we have an abstract gas of interacting particles with "position" coordinate ϕ_I^N and it is well known from classical mechanics that the centre of mass coordinate acquires the total mass of all particles as its effective mass, thus making it much heavier than the individual particles.

To see this in more detail, due to the above identity not all of the ϕ_I^N are independent. In case that the KG mass is small, the potential term in the Hamiltonian is well approximated by just the discretised Laplacian

$$-\frac{\delta_N^3}{\delta_N^2} \sum_I \phi_I \sum_{a=1}^3 (\phi_{I+\delta_a}^N + \phi_{I-\delta_a}^N - 2\phi_I^N) = \delta_N \sum_I \sum_a (\phi_{I+\delta_a}^N - \phi_I^N)^2$$
 (3.13)

which only depends on the relative coordinates. Here δ_a is the standard basis of \mathbb{R}^3 . It is thus motivated to choose new canonical variables $q_I:=\phi_I^N-\phi_0^N,\ I\neq 0$ and $\bar q:=\overline{\phi}$. Then with $A=N^3$ and $\phi_0^N=\overline{q}-\sum_{I\neq 0}q_n/A$ and the symplectic potential is

$$\frac{\theta}{\delta_N^3} = \sum_{I \neq 0} [\pi_I^N - \overline{\pi}] \ dq_n + [A\overline{\pi}] \ d\overline{q} \tag{3.14}$$

Thus the momentum conjugate to \overline{q} is the total momentum $P=\sum_n \pi_I^N=\overline{\pi}$ while $p_I=\pi_I^N-\overline{\pi}$ is conjugate to q_I . It follows $\sum_{I\neq 0} p_I=\overline{\pi}-\pi_0^N$ and twice the kinetic term in the Hamiltonian at finite cut-off is given by

$$\int d^3x \, \pi(x)^2 \approx \sum_{I} (\pi_I^N)^2 \, \delta_N^3 = \delta_N^3 \left[\frac{P^2}{A} + \sum_{n \neq 0} p_n^2 + (\sum_{n \neq 0} p_n)^2 \right]$$
 (3.15)

which displays the large total mass A of the centre of mass momentum P. A little bit of further analysis shows that the quadratic form of the p_I can be diagonalised by a a furher orthogonal transformation (which can be extended to a canonical one) displaying A-2 modes of unit mass and one mode of the "reduced mass" 1/A. Thus the centre of mass mode is indeed by far the heaviest d.o.f. especially in the limit $A \to \infty$.

One may object that the modes ϕ_I^N have nothing to do with the momentum modes $\hat{\phi}_I = < e_I, \phi >$ except for the zero mode $\hat{\phi}_0 = A\bar{q}$. However, this is not true because the ϕ_I^N are approximants of $\phi(x=\delta_N I)$, i.e. the field discretised on a lattice of the compact space given by the torus of volume L^3 . As is well known, in this situation, the Fourier transformation can also be restricted to the modes $k_I = k_L I = \frac{2\pi}{L} I, \ I \in \mathbb{N}_N^3$. We can in fact see this explicitly by writing

$$\phi_I^N = \frac{1}{L^3 \delta_N^3} \sum_{I' \in \mathbb{Z}^3} \langle e_{I'}, \chi_{N,I} \rangle \hat{\phi}_{I'}$$
 (3.16)

It is easy to see that the Fourier coefficients satisfy $< e_{I'}, \chi_{N,I} > = < e_{I'+lN}, \chi_{N,I} >$ for any $l \in \mathbb{Z}^3$ so that (take N even when taking $N \to \infty$ w.l.g.)

$$\phi_n^N = \frac{1}{L^3 \delta_N^3} \sum_{n' \in \mathbb{Z}_{N/2}^3} \langle e_{n'}, \chi_{N,n} \rangle \sum_{l \in \mathbb{Z}^3} \hat{\phi}_{n'+lN}$$
 (3.17)

where $\mathbb{Z}_{N/2}=\{-N/2,-N/2+1,..,N/2-1\}$. Thus, corresponding to the position space cutoff at δ_N we perform a momentum space cut-off at $Nk_L=2\pi/\delta_N$ and set $\hat{\phi}_{I'+lN}=0$ for $l\neq 0$. In the limit $N,n\to\infty,\ x=I\delta_N$ fixed, we recover the continuum relation $\phi(x)=\frac{1}{L^3}\sum_{I\in\mathbb{Z}^3}e_I(x)\ \hat{\phi}_I$. At finite N the (as one can show non-singular) matrix with matrix elements $< e_{I'},\chi_{N,I}>/\delta_N^3$ transforms between the position and momentum space discretisations.

In summary we have shown that the zero mode can be considered as a centre of mass mode with respect to certain linear combinations of discretised position modes which in turn are linear combinations of discretised momentum modes. The relation

$$\sum_{n \in \mathbb{N}_N^3} \phi_n^N / N^3 = \overline{\phi} = \langle e_0, \phi \rangle / L^3$$
(3.18)

remains exaxt also at finite N. Accordinly, treating the homogeneous mode as the by far most massive one is physically justifyable from this point of view. That instead of an arbitrarily large relative scale $1/N^3 \to 0$ we just used the finite one $\epsilon^2 = \kappa/\lambda$ is motivated by the specific combinations of the homogeneous momenta that appear in the Hamiltonian.

3.2 Quantum Cosmological SAPT

In order to understand the source of the problem originating from the infinite number of degrees of freedom, it is illustrative to consider a scalar field ϕ with conjugate momentum π coupled to Gaussian dust and General Relativity, that is model III described above. When gauge fixing the spacetime diffeomorphism gauge freedom the gravitational and scalar contribution to the Hamiltonian constraint combine to a physical Hamiltonian when integrated over the spatial slice [6]. All gravitational and scalar degrees of freedom now become observable fields. To simplify the model we switch off the inhomogeneous gravitational modes wrt a flat FRW background by hand. The Hamiltonian then takes the form

$$h = h_h(a, p, \phi_0, \pi_0) + h_i(\phi', \pi'; a), \quad h_i(\phi, \pi; a) := \frac{1}{2} \int_{\sigma} d^3x \left[\frac{\pi^2}{a^3} + a^3 \phi (\frac{-\Delta}{a^2} + m^2) \phi \right]$$
 (3.19)

with purely homogeneous contribution h_h whose precise form is not important for the purpose of this subsection and a contribution h_i which depends on the inhomogeneous scalar field modes (ϕ',π') as well as the scale factor a. Here p denotes the momentum conjugate to a, (ϕ_0,π_0) are the homogeneous scalar field modes and $\sigma\cong T^3$ is diffeomorphic to a 3-Torus of unit coordinate volume and Laplacian Δ . Note that the split (3.19) is not with respect to the adiabatic parameter.

When quantising h using the formalism of SAPT we are asked to work on the Hilbert space $\mathcal{H}=\mathcal{H}_f\otimes\mathcal{H}_s$. As far as the slow sector is concerned we will adopt a usual Schrödinger representation in accordance with the SAPT formalism. As h_i is quadratic in (ϕ',π') a Fock representation suggests itself, but which one? After all, the "background variable" a is not a fixed function of time but rather a dynamical variable which is in addution quantised, hence displays quantum fluctuations. The SAPT formalism enables us to consider a as a real parameter when quantising H_i with respect to the fast variables (ϕ',π') , hence it is natural to consider the Fock space $\mathcal{H}_f(a)$ with vacuum Ω_a and annihilation operator valued distribution symbol

$$b_a(x) := \frac{1}{\sqrt{2}} \left[\sqrt{\omega_a} \phi' - i \sqrt{\omega_a}^{-1} \pi' \right](x), \ \omega_a^2 = -\Delta a^2 + m^2 a^6$$
 (3.20)

where $x \in \sigma$ because then the a dependent normal ordering of H_i reads

$$h_i(a) = \frac{1}{a^3} \int_{\sigma} d^3x \ b_a^* \ \omega_a b_a \tag{3.21}$$

Then the excitations of Ω_a are obtained by applying the smeared creation operators

$$b_a(f)^* = \langle A_a, f \rangle = \int_{\sigma} d^3x \ A_a^* f$$
 (3.22)

where f is smooth.

Two immediate questions pose themselves:

1.

Are the corresponding Fock representations $(\rho_a, \mathcal{H}_f(a))$ of the (ϕ', π') all unitarily equivalent to a single one (ρ_f, \mathcal{H}_f) ? This is one of the innocent looking assumptions of SAPT which is automatically satisfied in the quantum mechanical context.

2

Assuming that this is the case, let $B(f) = W(b(f)), \ B^* = W(b(f)^*)$ be the Weyl quantisations of the symbols $b(f), b(f)^*$. Is the complete algebra of the operators $a, p, \phi_0, \pi_0, B(f), B(f)^*$ still well defined on $\mathcal{H}_f \otimes \mathcal{H}_s$?

It turns out that both questions are tightly related and surprisingly, the answer to both is negative. The underlying effect has been first observed in [9] in a related context. To see the origin of the problem, we note that a necessary condition for an affirmative answer to the first question is that the Fock vacuum Ω_{a_2} can be written as an excited state in \mathcal{H}_{a_1} for all a_1, a_2 ? In fact, this condition is also sufficient beccause polynomials of the $b_{a_1}(f)^*$ can be written as polynomials of the $b_{a_2}(f), b_{a_2}(f')$. Accordingly we make the Ansatz

$$\Omega_{a_2} = \sum_{N} z_N e_{a_1}(N) e_{a_1} = \prod_{I} \frac{[b_{a_1}(f_I)^*]^{N_I}}{\sqrt{N_I!}} \Omega_{a_1}$$
(3.23)

where I labels an orthornormal basis of inhomogeneous mode functions on σ

$$\langle f_I, f_J \rangle = \int_{\sigma} d^3x \, \overline{f_i(x)} \, f_J(x)$$
 (3.24)

and N denotes the collection of the occupation numbers N_I . The sum is over all N with only finitely many N_I different from zero. Then we impose $b_{a_2}(f_I)\Omega_{a_2}=0$ by using the Bol'ubov decomposition

$$b_{a_2} = \kappa_{+} b_{a_1} + \kappa_{-} b_{a_1}^{*}$$

$$\kappa_{\pm} = \frac{1}{2} \left[\sqrt{\frac{\omega_{a_1}}{\omega_{a_2}}} \pm \sqrt{\frac{\omega_{a_2}}{\omega_{a_1}}} \right]$$
(3.25)

As in our case all operators ω_a are mutually commuting we can pick the f_I to be eigenfunctions of $-\Delta$ with eigenvalues k_I^2 . Specifically on the torus the label set is $\mathbb{Z}^3-\{0\}$ and $k_I^2=(2\pi)^2||I||^2/L^2$ where L^3 is the volume of the torus. Let $\kappa_\pm(I)$ be the associated eigenvalues of κ_\pm and let δ_I be the the occupation number configuration $(\delta_I)_J=\delta_{IJ}$ then

$$0 = b_{a_{2}}(f_{I})\Omega_{a_{2}}$$

$$= \sum_{N} z_{N} \left[\sqrt{N_{I}} < f_{I}, \kappa_{+}f_{I} > e_{N-\delta_{I}} + \sqrt{N_{I}+1} < f_{I}, \kappa_{-}f_{I} > e_{N+\delta_{I}} \right]$$

$$= \sum_{N} \left[z_{N+\delta_{I}} \kappa_{+}(I)\sqrt{N_{I}+1} + z_{N-\delta_{I}} \kappa_{-}(I)\sqrt{N_{I}} \right] e_{N}$$
(3.26)

Since this hold for all I independently, the coefficients must be of infinite product type

$$z_N = \prod_I z_{N_I}^I \tag{3.27}$$

which transforms (3.26) into the recursion

$$z_{N+1}^{I} = -\sqrt{\frac{N}{N+1}} \sigma_{I} \ z_{N-1}^{I}, \ \sigma_{I} := \frac{\kappa_{-}(I)}{\kappa_{+}(I)}$$
(3.28)

where the r.h.s. vanishes for N=0. It follows $z_N^I=0$ for N odd while the solution of (3.28) for N is given by

$$z_{2N}^{I} = -\sqrt{\frac{2N-1}{2N}}\sigma_{I} \ z_{2(N-1)}^{I} = (-\sigma_{I})^{N} \sqrt{\frac{(2N)!}{4^{N}(N!)^{2}}} z_{0}^{I}$$
(3.29)

where z_0^I remains undetermined. It follows using manipulations well known from statistical physics

$$1 = ||\Omega_{a_{2}}||_{\mathcal{H}_{a_{1}}}^{2} = \sum_{N} |z_{N}|^{2} = \sum_{N} [\prod_{I} |z_{N_{I}}^{I}|^{2}] = \prod_{I} |z_{0}^{I}|^{2} ||\sum_{N=0}^{\infty} |z_{N}^{I}|^{2}]$$

$$= [\prod_{I} |z_{0}^{I}|^{2}] \prod_{I} [\sum_{N=0}^{\infty} \sigma_{I}^{2N} \frac{(2N)!}{4^{N}(N!)^{2}}]$$

$$\geq [\prod_{I} |z_{0}^{I}|^{2}] \prod_{I} [\sum_{N=0}^{\infty} (\frac{\sigma_{I}^{2}}{2})^{N}] = [\prod_{I} |z_{0}^{I}|^{2}] \prod_{I} (1 - \sigma_{I}^{2}/2)^{-1}]$$

$$\leq [\prod_{I} |z_{0}^{I}|^{2}] \prod_{I} [\sum_{N=0}^{\infty} \sigma_{I}^{2N}] = [\prod_{I} |z_{0}^{I}|^{2}] \prod_{I} (1 - \sigma_{I}^{2})^{-1}]$$

$$(3.30)$$

where the basic estimates $1 \geq (2N)!/(4^N(N!)^2) \geq 2^{-N}$ were used. Note that $\sigma(I) < 1$ so that the infinite product in the last step coming from the geometric series is meaningful. Thus a necessary condition for convergence of (3.30 is that the two infinite products converge independently to a finite, non zero value since $\prod_I z_0^I$ is a common prefactor in all z_N thus it must be convergent to some value Z by itself as otherwise all z_N would be meaningless. By taking the logarithm, the convergence of the second infinite product is equivalent to the convergence of the series

$$\sum_{I} \ln(1 - \sigma_I^2/2) \tag{3.31}$$

known as the Hilbert-Schmidt condition. We have with the abbreviation $\omega_j = \omega_{a_j}(I)$

$$\sigma_I^2 = \frac{\kappa_-(I)^2}{\kappa_+(I)^2} = \frac{\frac{\omega_1}{\omega_2} + \frac{\omega_2}{\omega_1} - 2}{\frac{\omega_1}{\omega_2} + \frac{\omega_2}{\omega_1} + 2}$$

$$= \left[\frac{\omega_1 - \omega_2}{\omega_1 + \omega_2}\right]^2 = \left[\left(\frac{\omega_1^2 - \omega_2^2}{(\omega_1 + \omega_2)^4}\right)^2 + \left[\left(\frac{(a_1^4 - a_2^4)k_I^2 + (a_1^6 - a_2^6)m^2)^2}{(\omega_1 + \omega_2)^4}\right]$$

$$= \left[\left(\frac{(a_1^4 - a_2^4)k_I^2 + (a_1^6 - a_2^6)m^2)^2}{(\omega_1 + \omega_2)^4}\right]$$
(3.32)

For large k_I we have $\omega_j \propto k_I a_j^2$ thus the fraction in 3.32) approaches a constant and the series in (3.31) diverges for any $a_1 \neq a_2$. On the other hand, note that if the coefficient in front of k_I^2 in ω_a^2 would not depend on a then σ_I^2 and thus $\ln(1-\sigma_I^2/2))$ would decay as $1/k_I^4$ and thus the series

$$\sum_{I} \ln(1 - \sigma_I^2) \tag{3.33}$$

would converge which would be sufficent for the convergence of (3.30) to a non zero value.

This answers the first question posed above. To see that the second question is equivalent to the first we note that given that a is represented as a self-adjoint operator A on the full Hilbert space \mathcal{H} , by the spectral theorem we may display the Hilbert space as a direct integral or Hilbert bundle subordinate to A

$$\mathcal{H} \cong \int_{\mathbb{R}_0^+}^{\oplus} d\mu(a) \,\mathcal{H}_a \tag{3.34}$$

where we identify the fibre spaces \mathcal{H}_a as the Fock spaces $\mathcal{H}_f(a)$ considered above and μ is the spectral probability measure on the spectrum of A which is $\sigma(A) = \mathbb{R}_0^+$. As a consequence of the spectral theorem the \mathcal{H}_a (of equal dimension) can be chosen identical [27] which we already know to be not the case but is instructive to pretend to not know this. Vectors in the Hilbert bundle are given by measurable fibre Hilbert space valued functions $\psi:\sigma(A)\mapsto\mathcal{H},\ a\mapsto\psi(a)$ over the base manifold $\sigma(A)$ and are equipped with the inner product

$$<\psi,\psi'> = \int d\mu(a) < \psi(a), \psi'(a) >_{\mathcal{H}_a}$$
 (3.35)

By the spectral theorem, A acts by multiplication by a in the fibre \mathcal{H}_a and accordinly the operator H_i acts fibre wise as well by the symbol $h_i(a)$ in (3.21). The question is now how the operator P representing p acts on the direct integral Hilbert space. As the spectrum of A is of absoltely continuous type, it acts as $P\psi = \psi'$ where $\psi'(a) = [i\hbar d/da + f(a)]\psi(a)$ where f(a) is related to the divergence of the measure μ and turns P into a symmetric operator (in fact, in order to obtain a self-adjoint operator one should pass to the real valued triad variable e and work with its conjugate momentum but the conclusion derived below is not affected by these sutleties). By contrast the operators B, $B^a st$ act fibre wise by the corresponding symbols.

It follows

$$[P,B] = i\kappa \cdot B^*, \ [P,B] = i\hbar K' \cdot B, \ \kappa'(a) = \frac{d}{da} \ln(\sqrt{\omega_a})$$
(3.36)

where K' is the Weyl quantisation of the symbol κ' and accordingly

$$B P \Omega = [B P] \Omega = -i\hbar K' \cdot B^* \Omega \tag{3.37}$$

which is solved by

$$P\Omega = -i\frac{\hbar}{2} \int_{\sigma} d^3x B(x)^* (K' \cdot B)^*(x) \Omega \tag{3.38}$$

The vector (3.37) has the norm

$$||P\Omega||^2 = \int_{\sigma(A)} d\mu(a) \, Tr_{L_2(T^3)}((\kappa'(a))^{\dagger} \kappa'(a))$$
(3.39)

which is finite only if the Hilbert-Schmidt norm

$$Tr_{L_2(T^3)}((\kappa'(a))^{\dagger}\kappa'(a)) = \sum_{I} |\langle f_I, \kappa'(a)f_I \rangle|^2 = \frac{1}{16} = \sum_{I} \left[\frac{\frac{d}{da}\omega_I(a)^2}{\omega_I(a)^2}\right]^2$$
 (3.40)

is finite μ a.e. We easily see that (3.40) is the infinitesimal version of (3.31) if we divide it by $(a_1 - a_2)^2$ and take the limit $a_2 \to a_1$.

Thus it is not possible to apply SAPT to the given Hamiltonian directly. One may think that by a different choice of Fock representations one maybe able to satisfy the Hilbert-Schmidt condition. However, if one wants to keep the correspondingly normal ordered Hamiltonian at least densely defined on Fock states then this again leads to an obstruction as one can show with more work.

To understand the origin of this obstruction, note that we can satisfy the Hilbert-Schmidt condition if we rescale the inhomogeneous degrees of freedom as

$$\tilde{\phi}' = a\phi', \ \tilde{\pi}' = \frac{\pi'}{a} \tag{3.41}$$

which still have canonical brackets and in terms of which we have

$$h_i = \frac{1}{2a} \int_{\sigma} d^3x \left[(\tilde{\pi}')^2 + \tilde{\phi}' \tilde{\omega}_a^a \tilde{\phi}' \right], \quad \tilde{\omega}_a^2 = -\Delta + m^2 a^2$$
 (3.42)

so that the coefficient of $-\Delta$ in $\tilde{\omega}_a^2$ is independent of a. However, (3.41) is not a canonical transformation on the full phase space so that it is no longer the case that $p, \tilde{\phi}', \tilde{\pi}'$ have vanishing Poisson brackets. Consequently, p cannot simply act on the a dependence of a wave function. One can of course complete the transformation (3.41) exactly by adding a corresponding contact term in the symplectic potential

$$\Theta = pda + \pi_0 d\phi_0 + \int dx \,\pi' d\phi' = \left(p - \frac{1}{a} \int dx \pi' \phi'\right) da + \pi_0 d\phi_0 + \int dx \,\tilde{\pi}' d\tilde{\phi}' \tag{3.43}$$

displaying

$$\tilde{p} = p - \frac{1}{a} \int dx \pi' \phi', \ \tilde{a} = a, \ \tilde{\phi}_0 = \phi_0, \ \tilde{\pi}_0 = \pi_0$$
 (3.44)

as the completion of that transformation. Unfortunately, now we have to write h_h in terms of \tilde{p} thereby introducing first and second powers of the (normal ordered) operator

$$\int dx \pi' \phi' = \int dx \tilde{\pi}' \tilde{\phi}' = \frac{i}{2} \int dx [\tilde{b}^2 - (\tilde{b}^*)^2 - 2\tilde{b}^* \tilde{b}]$$
(3.45)

Here \tilde{b} is the annihilator obtained from (3.20) by substituting all ingredients by those with a tilde. The operator (3.46) is obviously ill defined on the corresponding Fock space.

However, the discussion suggests to consider more general canonical transformations in order to avoid the desastrous terms such as (3.45). To restrict the class of such transformations we follow the logic of [9]: We remember that at present we are interested in perturbation theory with respect to the inhomogeneities up to second order in ϕ', π' which themselves are considered to be of first order. This suggests to restrict to transformations which are linear in ϕ', π' such as (3.41) since this keeps the second order nature of h_i and higher order transformations would anyway not be visible at the second order precision of h_i . The corresponding contact terms for the homogeneous degrees of freedom will then be already of second order in leading order as in (3.44) and we can restrict the precision of the canonical transformation to second order.

Correspondingly we consider transformations of the form (local in x)

$$\phi' = r \cdot \tilde{\phi}' + s \cdot \tilde{\pi}', \ \pi' = t \cdot \tilde{\phi}' + u \cdot \tilde{\pi}', \tag{3.46}$$

where r,s,t,u in principle can depend on all homogeneous degrees of freedom. Also all functions may involve a non-trivial (translation invariant - if we want to keep translation covariance) integral kernel (which is why we use the \cdot notation) and to satisfy the Hilbert Schmidt condition it will be sufficient to restrict it to be constructed from Δ so that they mutually commute and are symmetric on $L_2(T^3)$. Of course, r,s,t,u are restricted to be real valued since all variables are. In order that (3.46) be canonical taking only the Poisson brackets between ϕ',π' into account we must have

$$-t \cdot s + r \cdot u = 1_{L_t(T^3)} \Rightarrow u \cdot r - s \cdot t = 1_{L_t(T^3)}$$
 (3.47)

where the symmetry of the kernels was exploited and that $[r\cdot,s\cdot]=[t\cdot,u\cdot]=0$ due to mutual commutativity and

As before one now plugs (3.46) into the symplectic potential and computes the contact terms up to total differentials to second order in the perturbations. One then expresses the Hamiltonian in terms of the new variables, expands it to second order in the perturbations and determines the functions r, s, t, u such that the terms not densely defined on the Fock space cancel each other and such that the Fock spaces determined for different values of the homogeneous variables are all identical which will be the case if and only if the coefficient of $-\Delta$ in the corresponding frequency squared operator is independent of the phase space variables.

We will derive the completion of the canonical tranformation (3.46) abbreviating the homogeneous canonical pairs by $q^j, p_j, j = 1, 2$, using that convoluted kernels are also symmetric and dropping

total differentials as well as terms of fourth order in the perturbations

$$\begin{split} \Theta &= p_j dq^j + \pi' \cdot d\phi' = p_j dq^j + [t \cdot \tilde{\phi}' + u \cdot \tilde{\pi}'] \cdot d[r \cdot \tilde{\phi}' + s \cdot \tilde{\pi}'] \\ &= p_j dq^j + \tilde{\pi}' \cdot (u \cdot r - t \cdot s) \cdot d\tilde{\phi}' \\ &- \frac{1}{2} [\tilde{\phi}' \cdot d(t \cdot r) \cdot \tilde{\phi}' + \tilde{\pi}' \cdot d(u \cdot s) \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot d(t \cdot s) \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot dr) \cdot \tilde{\phi}' + \tilde{\phi}' \cdot (t \cdot ds + u \cdot dr) \cdot \tilde{\pi}' + \tilde{\pi}' \cdot (u \cdot ds) \cdot \tilde{\pi}'] \\ &= p_j dq^j + \tilde{\pi}' \cdot d\tilde{\phi}' \\ &- \frac{1}{2} [\tilde{\phi}' \cdot (t \cdot r)_{,q^j} \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s)_{q^j} \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot (t \cdot s)_{,q^j} \cdot \tilde{\pi}'] dq^j \\ &- \frac{1}{2} [\tilde{\phi}' \cdot (t \cdot r)_{,p^j} \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s)_{p_j} \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot (t \cdot s)_{,p_j} \cdot \tilde{\pi}'] dp^j \\ &+ [\tilde{\phi}' \cdot (t \cdot r_{,q^j}) \cdot \tilde{\phi}' + \tilde{\phi}' \cdot (t \cdot ds + u \cdot r_{,q^j}) \cdot \tilde{\pi}' + \tilde{\pi}' \cdot (u \cdot s_{,p_j}) \cdot \tilde{\pi}'] dp^j \\ &= \tilde{\pi}' \cdot d\tilde{\phi}' \\ &+ [p_j - \frac{1}{2} [\tilde{\phi}' \cdot (t \cdot r)_{,q^j} \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s)_{q^j} \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot (t \cdot s)_{,q^j} \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot r)_{,p^j} \cdot \tilde{\phi}' + \tilde{\phi}' \cdot (t \cdot ds + u \cdot r_{,q^j}) \cdot \tilde{\pi}' + \tilde{\pi}' \cdot (u \cdot s_{,q^j}) \cdot \tilde{\pi}'] dp^j \\ &= [-\frac{1}{2} [\tilde{\phi}' \cdot (t \cdot r)_{,p^j} \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s)_{q^j} \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot (t \cdot s)_{,q^j} \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot r)_{,p^j} \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s)_{p_j} \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot (t \cdot s)_{,p_j} \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot r)_{,p^j} \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s)_{p_j} \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot (t \cdot s)_{,q^j} \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot r)_{,q^j} \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s)_{q^j} \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot (t \cdot s)_{,q^j} \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot r)_{,q^j} \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s)_{q^j} \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot (t \cdot s)_{,q^j} \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot r)_{,q^j} \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s)_{q^j} \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot (t \cdot s)_{,q^j} \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot r)_{,q^j} \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s)_{q^j} \cdot \tilde{\pi}' + + 2\tilde{\phi}' \cdot (t \cdot s)_{,q^j} \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot r)_{,q^j} \cdot \tilde{\phi}' + \tilde{\phi}' \cdot (t \cdot ds + u \cdot r_{,q^j}) \cdot \tilde{\pi}' + \tilde{\pi}' \cdot (u \cdot s)_{,q^j} \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot r)_{,q^j} \cdot \tilde{\phi}' + \tilde{\phi}' \cdot (t \cdot ds + u \cdot r_{,q^j}) \cdot \tilde{\pi}' + \tilde{\pi}' \cdot (u \cdot s)_{,q^j} \cdot \tilde{\pi}'] \\ &+ [\tilde{\phi}' \cdot (t \cdot r)_{,q^j} \cdot \tilde{\phi}' + \tilde{\phi}' \cdot (t \cdot ds + u \cdot r_{,q^j}) \cdot \tilde{\pi}' + \tilde{\pi}' \cdot$$

whence to second order in the perturbations we have (use $u \cdot r - s \cdot t = 1_{L_2(T^3)}$

$$\tilde{q}^{j} = q^{j} - \frac{1}{2} [\tilde{\phi}' \cdot (t \cdot r_{,p_{j}} - r \cdot t_{,p_{j}}) \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s_{,p_{j}} - s \cdot u_{,p_{j}}) \cdot \tilde{\pi}'
+ \tilde{\pi}' \cdot (u \cdot r_{,p_{j}} - r \cdot u_{,p_{j}} + t \cdot s_{,p_{j}} - s \cdot t_{,p_{j}}) \cdot \tilde{\phi}'
=: q^{j} + x^{j} (q, p)
\tilde{q}^{j} = p_{j} + \frac{1}{2} [\tilde{\phi}' \cdot (t \cdot r_{,q^{j}} - r \cdot t_{,q^{j}}) \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot s_{,q^{j}} - s \cdot u_{,q^{j}}) \cdot \tilde{\pi}'
+ \tilde{\pi}' \cdot (u \cdot r_{,q^{j}} - r \cdot u_{,q^{j}} + t \cdot s_{,q^{j}} - s \cdot t_{,q^{j}}) \cdot \tilde{\phi}'
=: p_{j} + y_{j} (q, p)$$
(3.49)

Note that in deriving the conditions on r, s, t, u one must invert (3.46) and (3.49) only up to second order in $\tilde{\phi}', \tilde{\pi}'$ which themselves are considered as of first order. Thus

$$q^{j} = \tilde{q}^{j} - x^{j}(\tilde{q}, \tilde{p}), \ p_{j} = \tilde{p}_{j} - y_{j}(\tilde{q}, \tilde{p})$$
 (3.50)

so that up to second order

$$h_{h}(q,p) = h_{h}(\tilde{q},\tilde{p}) - \frac{\partial h_{h}}{\partial q^{j}}(\tilde{q},\tilde{p}) x^{j}(\tilde{q},\tilde{p}) - \frac{\partial h_{h}}{\partial p_{j}}(\tilde{q},\tilde{p}) y_{j}(\tilde{q},\tilde{p})$$

$$= \tilde{h}_{h} - \frac{1}{2} [\tilde{\phi}' \cdot (t \cdot \dot{r} - r \cdot \dot{t}) \cdot \tilde{\phi}' + \tilde{\pi}' \cdot (u \cdot \dot{s} - s \cdot \dot{u}) \cdot \tilde{\pi}' + \tilde{\pi}' \cdot (u \cdot \dot{r} - r \cdot \dot{u} + t \cdot \dot{s} - s \cdot \dot{t}) \cdot \tilde{\phi}'$$

$$(3.51)$$

where all functions on the r.h.s. are evaluated at \tilde{q},\tilde{p} and we used the abbreviation $\dot{r}=\{h_h,r\}$ etc. Next we note that in (3.46) we may replace r(q,p) by $r(\tilde{q},\tilde{p})$ when substituting into h_i since the corrections would be at least of fourth order since h_i is already of second order. Accordingly from (3.19) with $f=a^{-3},\;\omega^2=g(-\Delta)+k,g=a,\;k=m^2a^3$ in which we can also replace a by \tilde{a}

$$h_{i} = \frac{1}{2} [\tilde{\phi}' \cdot (t \cdot f \cdot t + r \cdot \omega^{2} \cdot r) \cdot \tilde{\phi}' \tilde{\pi}' \cdot (u \cdot f \cdot u + s \cdot \omega^{2} \cdot s) \cdot \tilde{\pi}' + 2\tilde{\pi}' \cdot (u \cdot f \cdot t + s \cdot \omega^{2} \cdot r) \cdot \tilde{\phi}']$$
(3.52)

where all functions depend on \tilde{q}, \tilde{p} . Combining

$$h_h + h_i - \tilde{h}_h = \frac{1}{2}\tilde{\phi}' \cdot (t \cdot f \cdot t + r \cdot \omega^2 \cdot r - [t\dot{r} - r\dot{t}]) \cdot \tilde{\phi}'$$

+ $\tilde{\pi}' \cdot (u \cdot f \cdot u + s \cdot \omega^2 \cdot s - [u\dot{s} - s\dot{u}]) \cdot \tilde{\pi}'$
+ $\tilde{\pi}' \cdot (2u \cdot f \cdot t + 2s \cdot \omega^2 \cdot r - [u\dot{r} - r\dot{u} + t\dot{s} - s\dot{t}]) \cdot \tilde{\pi}'$] (3.53)

The last term is ill defined on any Fock space, hence its round bracket must vanish. Denote the round bracket of the second term by $l\cdot l$ which is supposed to be positive and is allowed to be a function of both q,p and $-\Delta$. Then we wish that the round bracket of the first term takes the form $l(-\Delta+\tilde{m}^2)l$ where \tilde{m}^2 is a function of the homogeneous variables to be determined. This will guarantee that we can factor out l^2 from the expression of the Hamiltonian, leaving us with a Hamiltonian density of standard form with constant coefficients of $-\Delta$ so that the Hilbert-Schmidt condition is satisfied.

The simplest choice of r,s,t,u is such that 1. none of them depends on $-\Delta$ and 2. also l does not depend on $-\Delta$. This choice is in fact unique. Namely the expression for l and our assumption implies that s=0 and hence $r\cdot u=1_{L_2(T^3)}$. The round bracket in the second term is then $l\cdot l=u\cdot f\cdot u$ which is manifestly positive. Then the condition that the round bracket in the last term vanishes can be solved algebraically

$$t = -l^{-1} \cdot \dot{u} \cdot l^{-1} \tag{3.54}$$

which leads to the final condition

$$l \cdot (-\Delta + \tilde{k}) \cdot l = u^{-1} \cdot (l^{-1} \cdot \dot{u} \cdot u \cdot l^{-1} + \omega^2 + \{h_h, u \cdot t\}) \cdot u^{-1}$$
(3.55)

Again using the assumption we must match the coefficients of $-\Delta$ on both sides and we find

$$u \cdot l \cdot l \cdot u = u \cdot u \cdot f \cdot u \cdot u = g \tag{3.56}$$

which for the present model has the unique positive solution $u=\tilde{a}$ and thus $l^2=\tilde{a}^{-1}$. The transformed mass term becomes

$$u \cdot l \cdot \tilde{k} \cdot l \cdot u = l^{-1} \cdot \dot{u} \cdot \dot{u} \cdot l^{-1} + k - \{h_h, u \cdot l^{-1} \cdot \{h_h, u\} \cdot l^{-1}\}$$
(3.57)

To summarise:

We were indeed able to make the Hamiltonian symbol well defined on the same Fock space for all values of the homogeneous degrees of freedom. But the price to pay is twofold:

Due to the dependence of the mass term \tilde{k} displayed in (3.57) on both \tilde{q}, \tilde{p} , the BOA method is no

longer available. We are forced into its generalisation, the SAPT scheme.

2.

The mass term is not manifestly positive, it is generically indefinite and there is no freedom left to change this without making the coefficients r, s, t, u also depend on $-\Delta$. Whether this can be improved by exploiting the complete freedom in thos coefficients will be left for future research. 3.

In this respect, we draw the attention of the reader to reference [26]. There the starting point is indeed a Hamiltonian of second order in the inhomogeneous degrees of freedom with standard form up to a prefactor depending on the homogeneous degrees of freedom, except that the mass squared is a generic function of the homogeneous degrees of freedom. The Mukhanov-Sasaki Hamiltonian is a prominent example. Hence we are precisely in the situation arrived at above after our canonical transformation (exact up to second order). The analysis of [26] investigates the most general Fock representation, labelled by the homogeneous variables, that supports such a Hamiltonian and at the same time provides a canonical transformation of the homogeneous sector to variables which directly commute with the associated annihilation and creation variables. This has the adavantage that the Hilbert-Schmidt condition is trivially solved because the annihilation and creation operators do not depend on the transformed homogeneous degrees of freedom. As such, the strategy is similar in spirit to the present one although the details are different. One finds that in this case an algebraic solution is no longer possible, rather one must solve a system consisting of two non-linear (but semilinear) first order PDE's for complex coefficient operators coming from the Hamiltonian vector field of h_h to guarantee that all conditions are met, including the positivity of the mass term. One of the conditions is equivalent to the fixed point equation of the adiabatic vacua construction [8], the other determines an otherwise free phase. While those PDE's are well posed and can be solved in principle by the method of caracteristics, it is generically very hard to to solve the system explicity given the detailed form of h_h which, however, is a prerequisite to quantise the homogeneous sector as well. Thus for the purpose of the papers in this series, we stick to the method sketched above, although the possibility to guarantee the positivity of the mass squared term using the methods of [26] is very attractive in view of the complications that arise for negative mass squared terms discussed in the next subsection.

There is is also another, independent reason for why the approach of [26] is especially attractive: Since annihilation and creation operators commute with the operators of the homogeneous sector, the latter operators preserve the domain of the inhomogeneous part of the Hamiltonian. This is not necessarily the case when just guaranteeing the Hilbert-Schmidt condition. To see this suppose that the symbol κ' in (3.36) is of Hilbert-Schmidt type and only depends on a, then the vector $H_iP\Omega$, $H_i=W(h_i)$ is given by (recall (3.38)

$$H_i P \Omega = -i\hbar \int_{\sigma} d^3 x B(x)^* (\hat{\omega} \cdot K' \cdot B)^*(x) \Omega \tag{3.58}$$

but the symbol of $\hat{\omega} \cdot K'$ is up to a factor given by $\omega(a) \frac{d}{da} \ln(\omega(a)) = d\omega(a)/da$ which decays only as k_I even if the coefficient of $-\Delta$ in $\omega(a)^2$ is independent of a. By itself this is not a problem because we want to consider the spectrum of H = W(h) rather than $W(h_i)$ which does not require to have the commutator $[P, H_i]$ defined on the Fock space, however, it would be a convenient property to have (recall that once H can be constructed as a self-adjoint operator the existence of a dense and invariant domain is granted [27]) Again, to have a domain left invariant by the operators of the homogeneous sector could possibly granted within the context of this paper if we considered general r, s, t, u and in particular make the derivative of the function $l \cdot (-\Delta + M^2) \cdot l$ with respect to the homogeneous variables decay at least as k_I .

In view of this discussion we hope to come back to the formalism of [26] adapted to the present context in a future publication.

3.3 Indefinite mass squared operators

The discussion of the previous section applies to rather generic second order Hamiltonians. More generally one may have several matter or geometry species e.g. scalar, vector, tensor and spinor modes [28]. We can apply for each inhomogeneous species an individual canonical transformation parametrised by r_s, s_s, t_s, u_s where s labels the species and transform the symplectic potential for each of the species simulatenously the effect of which is that simply the x_s^j, y_j^s corrections for all species add up. Since we perturb h_h only linearly in x^j, y_j and since in each second order Hamiltonian we can drop the x^j, y_j corrections, the species contributions never mix up to second order perturbation theory.

Accordingly we can consider the hamiltonian symbols to be well defined on the corresponding Fock spaces and the Hilbert-Schmidt conditions are all solved. However, as concluded in the previous subsection, the mass squared terms M_s^2 for each of the species are generically not positive on the entire phase space. In what follows we present several strategies for how to deal with this problem, none of which is entirely satisfactory as they either lead to instabilities or contain ad hoc elements. Since this is a new situation, the discussion will be mostly exploratory.

- 1. One could exploit the full freedom in those transformations beyond the restricted Ansatz of the previous subsection to try to make positivity manifest. This possibility will be explored elsewhere. In that respect it should be mentiooned that there seems to be substantial freedom in the choice of the functions u, r, s, t and thus the regime of the phase space where the mass squared functions become negative depends on that freedom. In that sense, that region should not be of any physical significance and it would be most natural to get rid of it, thus restricting the freedom in the choice of the canonical transformations by a physically motivated criterion.
- 2. One could restrict the classical phase space of the homogeneous degrees of freedom to the set of points (q,p) where $M_s^2(q,p) \geq 0$ for all s. This restriction can be achieved by definining new variables v_s and to set $v_s^2 = M_s^2$. An especially nice situation is when the the M_s^2 have mutually vanishing Poisson brackets between them as we then can consider them as action variables and determine the corresponding angle variables as conjugate ones. This is in particular possible for a single field species as in (3.19) but already fails when we have tensorial and scalar field modes present at the same time. More generallly, we may be able to write M_s^2 in the form

$$M_s^2(q,p) = F_s^2(q,p)N_s^2(q,p)$$
(3.59)

where now $F_s(q,p)$ is a real function and N_s^2 is still indefinite but the N_s^2 are mutually commuting for all s for which N_s^2 is indefinite. Then we may apply the action angle prescription to $v_s^2=N_s^2$ (assuming that the number of homogneous pairs is at least as large as the number of indefinite mass squared terms). In the most general case we solve the equations $v_s^2=M_s^2(q,p)$ for some homogeneous momenta $p_s=F_s(v,c;z)$ (this may involve choosing branches) where c is the collection of the q^s conjugate to the chosen p_s and z stands for the remaining canonical pairs. The variables v,c,;z then coordinatise a new phase space with induced symplectic structure and while they are not canonical coordinates for it, they are supposed to have full range in some \mathbb{R}^{2m} in contrast to the p_s . We then must pass to suitable Darboux coordinates and hope that they are global in order that we may apply Weyl quantisation.

To illustrate this, we compute the mass squared opertor for the model (3.19) for which the homogeneous piece of the Hamiltonian reads (c is a positive constant)

$$h_h = -c\frac{p^2}{a} + \Lambda a^3 + \frac{1}{2}(\frac{\pi_0^2}{a^3} + m^2 a^3 \phi_0^2)$$
(3.60)

It follows

$$\dot{a} = \{h_h, a\} = -2c\frac{p}{a}, \ \dot{p} = \{h_h, p\} = -c\frac{p^2}{a^2} - 3\Lambda a^2 + \frac{3}{2}(\frac{\pi_0^2}{a^4} - m^2 a^2 \phi_0^2)$$
 (3.61)

Thus from (3.57) with $u = a, f = a^{-3}, l \cdot l = a^{-1}$

$$a\tilde{k} = \frac{\dot{v}^2}{9v} + m^2v - \frac{\ddot{v}^3}{v} = a^3 \tag{3.62}$$

we find

$$\tilde{k} = \left[m^2 - 6c\Lambda - 3cm^2\phi_0^2\right]a^2 + 3c\frac{\pi_0^2}{a^4} - 2c^2\frac{p^2}{a^2}$$
(3.63)

which is clearly indefinite. To illustrate more clearly the procedure, suppose that we would have treated the homogeneous mode of the scalar field on equal footing with the inhomogeneous ones so that the ϕ_0, π_0 dependent terms are missing from (3.60) and thus (3.63) which however is still indefinite even for tiny cosmological constant so that $M^2 := m^2 - 6c\Lambda > 0$. We define a new canonical pair $(b,q) \in \mathbb{R}^2$ and functions a,p of b,q by (set $\delta^2 := 2c^2/M^2$)

$$a^2 := b^2 + \delta^2 \frac{q^2}{b^2}, \ p := \frac{a}{b}q$$
 (3.64)

Note that in cosmology a>0 so that the square root in (3.64) has only one branch and thus (3.64) is uniquely defined away from b=0. To see that this is locally a canonical transformation we compute

$$\{p,a\} = \{\frac{a}{b}q,a\} = a\{\frac{q}{b},a\} = \frac{1}{2}\{\frac{q}{b},a^2\} = \frac{1}{2}\{\frac{q}{b},b^2 + \delta^2(\frac{q}{b})^2\} = \frac{1}{2b}\{q,b^2\} = 1$$
 (3.65)

and thus

$$\tilde{k} = M^2 b^2 \tag{3.66}$$

is manifestly positive. However, (3.64) restricts the original range $(a,p) \in \mathbb{R}_+ \times \mathbb{R}$ to the set of pairs (a,p) with $a^4 > \delta^2 p^2$, $p \in \mathbb{R}$.

In general, even if possible, the canonical transformations involved worsen the degree of non-polynomiality of the symbol h(z) with respect to the homogeneous degrees of freedom z=(q,p).

3. The third possibility to is to take the indefinite mass terms k seriously as the stand. Accordingly, for certain ranges of the homogeneous variables (q,p) the inhomogeneous symbol h_i defines a quantum field theory of tachyons! A possibility to deal with the tachyonic instabilty was suggested in [18]: We construct the Fock space $\mathcal{H}_{(q,p)}$ as before but we only allow those modes corresponding to eigenfunctions f_I , $I\mathbb{Z}^3-\{0\}$ of $-\Delta$ witheigenvalue $k_I^2+\tilde{k}(q,p)\geq 0$. Accordingly, the more negative \tilde{k} becomes the larger the infrared cut-off on the admissable modes. Specifically, for the example (3.63) with $\phi_0=\pi_0$ we find that \tilde{k} gets very negative for $p^2/a^2\to\infty$. If we interprete this as $\propto \dot{a}^2$ and take a baryon or radiation dominated universe then this certainly diverges at the classical big bang.

For the SAPT theory this has the following consequence:

If we take a torus of length L in all directions then $k_I^2=k_L^2||I||^2,\ k_L=2\pi/L.$ Let z=(q,p) and $\tilde{k}(z)$ be the indefinite mass squared term. Let S_\pm be the subsets of the slow phase space defined by $\tilde{k}(z)\geq 0$ and $\tilde{k}(z)<0$ respectively. We can enumerate the spectrum $E_n(z)$ of the Hamiltonian symbol $h_(z)$ by a mode number M, positive intergers $N_1,..,N_M$ and mutually distinct positive numbers $r_1<...< r_M$ with $r_k=||I_k||,\ I_k\in\mathbb{Z}^3-\{0\}.$ The spectral value is given by

$$E_n(z) = \sum_{k=1}^{M} N_k \sqrt{k_L^2 r_k^2 + \tilde{k}(z)}$$
 (3.67)

The mode number configurations which give rise to the same $E_n(z)$ determine the degeneracy of $E_n(z)$. First we see that varying the M,N_k,r_k does not leave (3.67) invariant (a.e. wrt z) as otherwise the numbers $\sqrt{k_L^2r^2+\tilde{k}(z)}$ would be linearly dependent over the positive

rationals which is not the case a.e. It follows that the only degeneracy lies in choosing the I_k with given r_k for which there are 8 possibilities, thus the degenracy of $E_n(z)$ is 8^M with $n=n(M,\{N_k\},\{r_k\})$ independent of z when $z\in S_+$.

However, for $z\in S_-$ we compute $r(z)^2:=-\tilde{k}(z)$ and can only allow the energy band n with $r_1\geq r(z)$. It follows that the eigenvalue $E_n(z)$ simply does not exist when $r_1< r(z)$. Consequently, also the eigenstates $e_n(z)$ and the standard vectors b_n that enter the Moyal projectors and unitarities $\pi_{n,0}(z), u_n(z)$ are simply deleted, the Fock space $\mathcal{H}_f(z)$ is the subspace of \mathcal{H}_f spanned by the $e_n(z)$ with $r_1\geq r(z)$. In other words, the function $z\mapsto E_n(z)$ for given n has a discontinuity at the surface $r_1=r(z)$ in the phase space. This can be problematic when computing the the Moyal products which ask to take derivatives with respect to z, a possibility being to take the one sided derivatives only.

- 4. In an ad hoc manner, one could restrict the phase space integral that enters the Weyl quantisation to S_+ , i.e. one multiplies all symbols such as h(z) with $\chi_{S_+}(z)$ where $\chi_{S_+}(z)$ denotes the characteristic function of S_+ . This is again not differentiable and thus it would be more appropriate to substitute χ_{S_+} by a mollified version of it (i.e. a smooth function that is zero in S_- and smoothly reaches unity within S_+ in an arbitrarily small neighbourhood of the boundary ∂S_+) in order that the Moyal product is meaningful. Of course, the quantum theory then will depend on that mollification which introduces ambiguities and technical challenges as the mollifier is a highly non polynomial function of z.
- 5. We could consider a mode decomposition of $h_i(z)$ and for $z \in S_-$ write $h_i(z) = h_i^+(z) + h_i^-(z)$ where h_i^+ is the contribution from all modes I with $k_I^2 \geq r(z)$. Then $h_i^+(z)$ is quantised as before and $h_i^-(z)$ is a finite sum of flipped harmonic oscillators of the type $p^2 \omega^2 q^2, \omega^2 > 0$. The difference with item [3.] is that we do not discard h_i^- . The spectrum of a flipped harmonic oscillator is purely of the absolutely continuous type [16] and thus the spectrum of $h_i(z)$ is drastrically changed when we transit from S_+ to S_- with corresponding consequences for the SAPT scheme. Besides, such a theory would be unstable.

For the model (3.19) strategy [2.] seems to be most promising as we will see in another paper of this series.

3.4 Non-polynomial operators

The purely homogeneous piece h_h of the Hamiltonian is non-polynomial in the scale factor a and contains inverse powers of it. The mass squared corrections coming from the canonical transformation performed in section (3.2) contains derivatives of h_h and increases that negative power. Furthermore, the adiabatic corrections contain additional derivatives of h_h of aribtrary order coming from the Moyal product and thus introduces furteher arbitrarily negative powers of a. Even worse, after the mass squared corrections we potentially also find inverse powers of arbitrarily high order in the momentum p conjugate to a, the Mukahnov Sasaki mass term being a prominent example.

It transpires that it would be desirable to have at one's disposal a dense set of vectors which is invariant under any of the operators corresponding to $a^n, p^n, n \in \mathbb{Z}$. In LQC one deals with negative powers of a by using a representation inspired by the representation used in the full LQG theory such that the spectrum of a is pure point rather than absolutely continuous and thus a commutator between fractional powers of a and Weyl elements for p is both densely defined and introduces the desired negative powers a. This comes at the price that the operator corresponding to p does not exist and one thus needs to approximate it by polynomials in Weyl elements. However, negative powers of p would then also need to be approximated by inverse polynomials of Weyl elements and these are not in the domain of a so that for our purpose the representation chosen in LQC is of no direct advantage.

We thus advocate to take an unbiased point of view and ask whether it is possible to choose the above desired domain directly in the Schrödinger representation, the advantage being that the operators corresponding to a,p exist. We found the following answers:

Theorem.

Let $\mathcal{H} = L_2(\mathbb{R}, x)$ be the Schrödinger representation of q, p as operators $(Q\psi)(x) = x\psi(x)$, $(P\psi)(x) = id\psi(x)/dx$. i.

There exists a dense and invariant domain D for the operators Q^n P^m , $n \in \mathbb{Z}$, $m \in \mathbb{N}_0$ consisting of smooth functions of rapid decrease both at x = 0 and at $x = \pm \infty$.

D is spanned by functions b_n , $n \in \mathbb{Z}$ whose inner products can be computed analytically in closed form. Correspondingly an orthonormal basis can be be constructed by the Gram-Schmidt procedure.

iii.

Let F be a function such that F^{-1} is a polynomially bounded function both in terms of x and x^{-1} and smooth except possibly at $x = 0, \pm \infty$. Let $f_1, ..., f_N$ be polynomials in x. Then there exists a common domain $D_L(F) \subset D$ for the operators of item i. and of the operators corresponding to the symols $|F(q)|^2 f_k(q)p^{-k}$, k = 1, ..., N in suitable symmetric orderings where L depends on both N and the degree of the polynomials f_k .

The proof of this theorem can be found in [25]. Note that P^{-1} is a symmetric operator with distributional kernel

$$(P^{-1}\psi)(x) = -\frac{i}{2\hbar} \int_{\mathbb{R}} dy \operatorname{sgn}(x-y)\psi(y)$$
(3.68)

The domain of P^{-1} must be carefully chosen: Even if ψ is a Schwartz function, while $P^{-1}\psi$ is smooth, it may not be of rapid decrease any more at infinity. Likewise, it is a simple collary that a dense and invariant domain for P^nQ^m , $n\in\mathbb{Z}$, $m\in\mathbb{N}_0$ is given by the Fourier transform of the functions of item i. but that Fourier transform is not necessarily of rapid decrease in x any more. This is why the statement of item iii. is significantly weaker, in particular, $D_L(F)$ is not an invariant domain for the list of operators stated and it is presently not clear whether it is dense. It is however certain that there exists no function in D orthogonal to $D_L(F)$.

The idea for defining the rather singular symbols that we encounter in the homogeneous sector of quantum cosmology is thus as follows (provided that we can factor out a suitable $|F|^2$ as described above): At any order of the adiabatic expansion the terms that involve negative powers of p are of the form described in item iii. and are finite in number. Thus we use the ordering alluded to in item iii. and the domain described there. The other terms not involving negative powers of p are also defined on that domain since $D_L(F) \subset D$.

4 Conclusion and Outlook

In the present first paper of this series we provided the tools with which we will intend to improve on the treatment of backreations in quantum cosmology. Thus we prepared the ground to approach the various models that are being treated in the subsequent papers of the series.

The plan of the subsequent papers in this series is as follows:

In the second paper [29] we treat the two quantum mechanical models labelled as models I and II in section 3.2. Model I is a standard QM problem consisting of polynomially coupled slow anharmonic and fast harmonic oscillator which mimicks the situation of model II and serves to illustrate the formalism. Model II considers the purely homogeneous cosmological sector, i.e. homogeneous geometry coupled to a homogeneous inflaton. In suitable variables this model can be dispalyed as an inverted slow harmonic oscillator non-polynomially coupled to a fast standard harmonic oscillator. The adiabatic parameter squared is here the ratio of coupling constants for gravity and the inflaton which we assume to be very small. The adiabatic parameter can also be written as the ratio of corresponding inflaton and Planck mass scales and thus is very tiny if we consider the latter to be of

the order of the mass scales that appear in the current standard model of elementary particle physics. That parameter will also organise the adiabatic perturbation expansion of the third and fourth paper.

In the third paper [30] we consider as matter content an inflaton and Gaussian dust. The usual Hamiltonian constraint is now a physical Hamiltonian as shown in [6] and the full constraints, not only their perturbations are already solved, all metric and inflaton degrees of freedom are physical observables. We expand the physical Hamiltonian to second order in the inhomogeneous modes leading to three scalar, one vector and two tensor modes. For simplicity we consider only quantisation of the inflaton field, i.e. we drop all metric perturbations and keep only the homogeneous metric degrees of freedom.

Finally in the fourth paper [31] we consider as matter content just the inflaton field and follow closely [9] in order to extract the gauge invariant observables of which there is the Mukhanov-Sasaki field and the tensor mode (primordial gravitational wave).

In all papers we compute the backreaction effects to second order in the adiabatic parameter thus displaying their existence and potential phenomenological importance that we will explore in a forthcoming publication. Note that the model of the second paper can be considered as the purely homogeneous truncation of both the model of the third and the fourth paper respectively, just that in the first case it is to be considered as a dynamical system with true Hamiltonian, in the second case that Hamiltonian is constrained to vanish. Accordingly, for the second paper we are interested in the full spectrum of the Hamiltonian which in appropriate variables can be considered as a harmonic oscillator non-polynomially coupled to an inverted harmonic oscillator [16].

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