Initial conditions and backreaction effects in quantum cosmology

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Abstract

The present thesis addresses the problem of cosmological backreaction, i.e., the question of whether and to which extent cosmological inhomogeneities affect the global evolution of the Universe. We will thereby focus on, but not restrict to, backreaction in a purely quantum theoretical framework which is adapted to describe situations during the earliest phases of the Universe. Our approach to evaluating backreaction uses a perturbative and constructive mathematical formalism which is denoted as space adiabatic perturbation theory, and which extends the well–known Born–Oppenheimer approximation to molecular systems.

The underlying idea of this scheme is to separate the system into an adiabatically slow and a fast part, similar to the separation of nuclear and electronic subsystems in a molecular setting. Such a distinction is reasonable if a corresponding perturbation parameter can be identified. In case of molecular systems, such a parameter arises as the ratio of the light electron and heavy nuclear masses. In the case of the here considered cosmological systems, we identify the ratio of the gravitational and the matter coupling constants as a suitable perturbative parameter. In a first step, we apply the space adiabatic formalism to a toy model and compute the backreaction of a homogeneous scalar field on a homogeneous and isotropic geometry. We restrict the computations to second order in the adiabatic perturbations and obtain an effective Hamilton operator for the geometry.

In the sequel, we apply space adiabatic perturbation theory to an inhomogeneous cosmology and calculate backreaction effects of the inhomogeneous quantum cosmological fields on the global quantum degrees of freedom. Therefore, it is necessary to first extend the scheme adequately for an application to infinite dimensional field theories. In fact, the violation of the Hilbert–Schmidt condition for quantum field theories prevents a direct application of the scheme. A solution is obtained by a transformation of variables which is canonical up to second order in the cosmological perturbations. This allows us to compute an effective Hamilton operator for a cosmological field theory previously deparametrized by a timelike dust field as well as the identification of an effective Hamilton constraint for a system with gauge–invariant cosmological perturbations. Both objects act on the global degrees of freedom and include the backreaction of the inhomogeneities up to second order in the adiabatic perturbation theory.

We conclude that it is a priori inadmissible to neglect cosmological backreaction. However, due to the general difficulties associated with finding solutions for coupled gravitational systems, the concrete evaluation of the operators found here must remain the subject of future research. One obstacle is the occurrence of indefinite mass squares associated with the perturbation fields which are the result of the previous transformations (which however, already appear in independent problems, for example in the use of Mukhanov–Sasaki variables) . A further complication in the final quantization and search for appropriate solutions arises from the non–polynomial dependence on the global degrees of freedom. We discuss these obstacles in detail and point to possible solutions.

Zusammenfassung

Die vorliegende Dissertation befasst sich mit dem Thema der kosmologischen Rückwirkungen, also insbesondere der Frage ob und in welchem Ausmaße kosmologische Inhomogenitäten die Entwicklung des Universums auf seinen größten Skalen beeinflusst. Dabei liegt unser Fokus auf Rückwirkungen in einem rein quantenmechanischen Formalismus, welcher mutmaßlich das Universum in seinen frühesten Phasen adäquat beschreibt. Wir werden allerdings ebenso auf Resultate und den Forschungsstand auf dem Gebiet der Rückreaktionen für die späteren semiklassischen und klassischen Phasen eingehen. Unser Ansatz zur Berechnung von quantenmechanischen Rückwirkungen beruht auf der perturbativen und konstruktiven Raumadiabatischen Störungstheorie, welche eine Erweiterung der bekannten Born–Oppenheimer Approximation für molekulare Systeme darstellt.

Die Idee des verwendeten Schemas beruht darauf das betrachtete Gesamtsystem in einen adiabatisch langsamen und einen schnellen Anteil zu separieren, ähnlich wie die Unterteilung in Kern– und Elektronensysteme auf molekularer Ebene. Dies ist dann physikalisch sinnvoll, wenn ein entsprechender Störparameter identifiziert werden kann. Im Falle von molekularen Systemen ist dies das Massenverhältnis; im Falle der hier betrachteten kosmologischen Systeme identifizieren wir das Verhältnis der gravitationellen und der Materie–Kopplungskonstanten als Störparameter. In einem ersten Schritt wenden wir die Raumadiabatische Störungstheorie auf ein einfaches Beispielsystem an und berechnen die Rückwirkung eines homogenen Skalarfeldes auf eine homogene und isotrope Geometrie. Wir beschränken uns dabei auf die Ermittlung eines effektiven Hamiltonoperators für die Geometrie bis zur zweiten Störungsordnung.

Im Weiteren wenden wir das Raumadiabatische Schema auf inhomogene kosmologische Systeme an und berechnen die Rückwirkungen der inhomogenen quantenkosmologischen Felder auf die globalen Quantenfreiheitsgrade des Systems. Dazu müssen wir das Schema zunächst adäquat für die Anwendung auf unendlich dimensionale Feldtheorien erweitern. Tatsächlich verhindert die Verletzung der Hilbert–Schmidt Bedingung für Quantenfeldtheorien die Anwendung des Schemas auf die hier betrachteten Systeme. Eine Lösung erhält man durch eine Variablentransformation der Feldtheorie, die hier bis auf zweite Ordnung in den kosmologischen Störungen kanonisch ist. Dies ermöglicht die Berechnung eines effektiven Hamiltonoperators für eine kosmologische Feldtheorie, die zuvor durch ein Staubfeld deparametrisiert wurde, sowie die Bestimmung einer effektiven Hamilton Zwangsbedingung für ein System mit eichinvarianten, kosmologischen Störungen. Beide Objekte wirken auf die globalen Freiheitsgrade und beinhalten die Rückwirkungen der Inhomogenitäten bis zur zweiten adiabatischen Störungsordnung.

Wir schließen daraus, dass es a priori unzulässig ist solche kosmologischen Rückwirkungen zu vernachlässigen. Aufgrund der allgemeinen Schwierigkeit Lösungen für gekoppelte gravitationelle Quantensysteme zu finden, muss allerdings die konkrete Auswertung der ermittelten Operatoren und Zwangsbedingungen Gegenstand zukünftiger Forschung bleiben.

Eine Hürde stellt dabei das Auftreten von indefiniten Massenquadraten für die Feldtheorien dar, die Resultat der zuvor durchgeführten Transformationen sind (welche aber auch schon in

hiervon unabhängigen Problemen auftauchen, zum Beispiel bei der Verwendung von Mukhanov–Sasaki Variablen). Ein Erschwernis bei der finalen Quantisierung und Suche nach entsprechenden Lösungen ergibt sich zudem durch die nicht–polynomielle Abhängigkeit von den globalen Variablen. Wir diskutieren diese Hürden ausführlich und weisen auf mögliche Lösungsstrategien hin.

Résumé

Cette thèse aborde le problème des réactions inverses en cosmologie. Plus précisément, nous cherchons à donner une réponse à la question de la signification et de la forme des effets excercés par les inhomogénéités cosmologiques sur l'évolution globale de l'Univers et cela dans un cadre purement quantique. Nous nous concentrerons donc, mais sans nous y limiter, sur les réactions inverses quantiques adaptées pour décrire les premières phases de l'Univers. Notre approche se sert d'un formalisme perturbatif et constructif nommé théorie des perturbations spatio–adiabatiques et qui s'inspire de l'approximation de Born–Oppenheimer bien connue de l'analyse spectrale des systèmes moléculaires. Cette théorie développe l'approche de Born–Oppenheimer de plusieurs façons.

L'idée sous–jacente de cette approche consiste à séparer le système en une partie adiabatiquement lente et en une partie rapide, similaire à la séparation des sous–systèmes nucléaires et électroniques dans un molécule. Une telle distinction est raisonnable si un paramètre perturbatif correspondant peut être identifié. Dans le cas des systèmes moléculaires, un tel paramètre provient de la fraction des masses des électrons légers et des noyaux lourds. En cosmologie par contre, nous identifions le rapport des constantes de couplage de la gravitation et de la matière comme un paramètre perturbatif susceptible. Dans une première étape, nous appliquons ce formalisme spatio–adiabatique à un modèle d'oscillateurs simples ainsi qu'à un modèle cosmologique réduit de symétries comprenant un champ scalaire couplé à la géométrie d'espace–temps. Nous réussissons à dériver des opérateurs hamiltonien effectifs dans les deux cas qui comprennent les réactions inverses du système rapide excercés au système lent. Nous nous limitons à des calculs au second ordre dans les perturbations adiabatiques.

Par la suite, nous appliquons la théorie des perturbations spatio–adiabatiques à des modèles de cosmologie inhomogène et calculons les effets des réactions inverses des champs cosmologiques quantiques et inhomogènes sur les degrés de liberté quantiques globaux (par exemple sur le taux d'expansion de l'Univers). Pour cela, il est nécessaire d'étendre le schéma de manière adéquate pour permettre son application aux théories des champs de dimension infinie. Plus précisément, la violation de la condition de Hilbert–Schmidt dans le contexte des théories quantiques des champs empêche l'application directe du schéma. Il s'avère qu'une transformation des variables (au niveau classique) qui est canonique jusqu'au second ordre dans les perturbations cosmologiques offre une solution à ce dilemme. Ces transformations nous permettent de calculer un opérateur hamiltonien effectif pour une théorie cosmologique des champs quantiques, préalablement déparamétrisée par un champ de poussière, ainsi que l'identification d'une contrainte hamiltonienne effective pour un système comprenant des perturbations cosmologiques invariantes de jauge. Les deux objets agissent sur les degrés de liberté globaux et incluent les effets des réactions inverses des inhomogénéités jusqu'au second ordre spatio–adiabatique.

Nous concluons par souligner qu'il est a priori inadmissible de négliger les effets de réaction inverse en cosmologie selon nos résultats. Cependant, en raison des difficultés générales associées à la recherche de solutions pour les systèmes gravitationnels couplés à la matière, l'évaluation

concrète des opérateurs trouvés ici reste le sujet de recherches futures. Un obstacle est l'apparition de carrés de masse indéfinis associés aux champs perturbatifs qui sont le résultat des transformations mentionnées ci–dessus. Une autre complication dans la quantification finale et la recherche de solutions appropriées provient de la dépendance non–polynomiale des degrés de liberté globaux. Nous discutons ces obstacles en détail et indiquons des solutions possibles.

Contents

Part I.

Introduction

1. Backreaction and the Physical Standard Model

The aim of this work is to investigate the physical interactions in the very early Universe and more precisely to develop a suitable theoretical formalism that incorporates backreaction effects between the different components of gravity–matter systems. In particular, we develop a formalism within non–perturbative quantum gravity that allows to iteratively include the interactions between its constituents while providing effective quantum constraints or equations of motion with a significantly simpler structure compared to full quantum gravtiy, and whose solutions become hence into reach. Progress in this direction will also allow to approach the semiclassical limit in quantum cosmology which is of utmost importance in order to bridge the gap between theory and experiment. The purpose of this introductory chapter is to motivate and specify the assumptions of this endeavor, to examine their adequacy, and to eventually provide the reader with a short outline of our goals and achievements.

We will first show how our specific research question is directly linked to the scientific progress in the fields of general relativity, the concordance model of cosmology, and the open questions related to it, the invention of quantum mechanics and the related perturbative quantum field theories, the technical difficulties arising in quantum field theories on curved space times and full non–perturbative quantum gravity. We will then present several strategies to mitigate the latter obstacles and bridge the gap between theory and observation. In particular, we shortly discuss several Planck mass perturbation theories, symmetry reduction, and the question of how the semiclassical limit of quantum gravity is related to our question of backreaction. The two former programs are however only partly able to solve these problems and neglect important parts of the interaction between the gravity and matter degrees of freedom. We therefore strongly advocate to apply the scheme of space adiabatic perturbation theory (SAPT) to quantum gravity, or our extension thereof, and point to the goals that have been achieved in the course of this thesis.

We refer the reader who is exclusively interested in acquiring information about the considerable advantages of implementing SAPT in perturbative quantum cosmology in comparison to other approaches studied so far, and who would like to jump to the specific achievements of this thesis, directly to section 1.1.10 of this chapter. Besides, more detailed overviews of certain topics can be found in part II of this thesis. Since we follow the development of the relevant theories in chronological order, this chapter can also be perceived as a historical synopsis. It provides the relevant notions necessary for this thesis but also goes beyond in that it offers a thorough historical embedding. A concise and more pragmatic outline of this thesis will be given in section 1.2.

1.1. Physical and Historical Background

To begin with, we clarify the meaning of the notion of "backreaction" used here, leading us directly to the theoretical foundations of this work and its embedding in 20th and 21st century physics. In particular, by backreaction we mean the effect of quantum cosmological perturbations (i.e., of quantized fields of linear cosmological perturbations) on the homogeneous quantum cosmological degrees of freedom of a gravity–matter system. This is of course not the only possible definition of backreaction as we will see in the sequel but it makes certainly sense to denote these effects as backreaction effects.

The backreaction problem is then concerned with the question about how and to which extent these backreactions from the perturbations possibly affect the background, and aims hence at incorporating the actual (or at least improved) dynamics of the system which has been (over–)simplified before. Here, we start however with the question of why this problem arises at all and how it is founded in the developments of physics during the last centuries. We take a step back and start with the inceptions of general relativity, quantum theory and quantum field theory on curved space time (QFT on CST).

1.1.1. The Success of General Relativity

Indeed, the 20th century started with a physical revolution regarding the common understanding of space and time especially brought forward by Einstein (1905b), (Weinberg 1972): In accordance with most experimental data at that time and following Newton's *Philosophiæ Naturalis Principia Mathematica*, most physicists and natural philosophers had assumed that all motions take place on a static three–dimensional Euclidean spatial manifold with a common uniform time variable. It was soon recognized that the induced Galilean space time transformations led to inconsistencies when applied to the famous Maxwell equations for electromagnetism but that another set of transformations which became known under the name of Lorentz transformations leaves them invariant (Larmor 1897; Lorentz 1904; Macrossan 1986; Poincaré 1905; Weinberg 1972). Thereupon, Einstein (1905b) derived the same transformations by assuming the principle of relativity and the constancy of the speed of light in all inertial frames, hence showing that the transformation of space and time coordinates of relatively moving inertial observers is provided by Lorentz' transformations (Weinberg 1972). As Minkowski (1909) realized, Einstein's special theory of relativity is most conveniently formulated by introducing four–dimensional space time vectors, and more generically in a covariant way in which the static Minkowski metric $\eta_{\mu\nu}$ is a constant Lorentz–invariant tensor field providing a measure of space and time for inertial observers (Einstein 1914).

Einstein and Grossmann (1913) finally succeeded in developing a likewise covariant theory of the gravitational force denoted as general relativity (see chapter 2 and particularly section 2.1) which replaces the constant Minkowski metric with a generally space time dependent metric tensor field $g_{\mu\nu}$ (Einstein 1914, 1916a; Weinberg 1972). The dynamical Einstein field equations for $g_{\mu\nu}$ depend directly on the distribution of the matter and energy content, and are given by $G_{\mu\nu} = 8\pi G\, T_{\mu\nu}$ where $G_{\mu\nu}$ is the geometric Einstein tensor, $T_{\mu\nu}$ is the matter stress–energy tensor and G is Newton's constant. Einstein's theory changed the understanding of space and time

severely. One relevant feature is that there is no preferred coordinate system and that physics must not depend on a coordinate choice, i.e., the theory is diffeomorphism invariant. Besides and most importantly, the *geometry of space time is dynamical* which is a very crucial feature for our backreaction problem here.

To date, general relativity presents one of the most successful physical theories whose foundations and implications could be tested up to very high precision at the scale of our solar system and below: Both the weak and the strong equivalence principle underlying the theory (Will 1993) could be checked and confirmed to the highest accuracy (Dittus and Lämmerzahl 2005). For example, Touboul et al. (2017) tested the universality of free fall (and hence the weak equivalence principle) with a precision to the order of 10^{-15} while Voisin et al. (2020) confirmed the strong equivalence principle with a pulsar in a triple stellar system. The recent detection of gravitational waves provides a meanwhile extensive catalog of different gravitational systems confirming Einstein's theory in an additional astonishing way (B. P. Abbott et al. 2019; R. Abbott et al. 2020). In fact, Einstein (1916a) himself had already deduced the anomalous precession of the perihelion of Mercury and thus presented a first important test of his theory by explaining already existing experimental data (Le Verrier 1859). In short, general relativity is one of the best tested scientific theories, at least on scales of the solar system (Will 2006), and predicts a plethora of physical phenomena that have been detected today such as black holes (Ghez et al. 1998; Schwarzschild 1916) and gravitational waves (B. P. Abbott et al. 2019; Einstein 1916b, 1918).

1.1.2. Our Universe and Concordance Cosmology

Unfortunately, Einstein's equations are second order, non–linear differential equations for the metric tensor and consequently very difficult to solve. Exact solutions only exist for very specific, highly symmetric situations such as black holes (Townsend 1997) or for cosmological symmetries (Stephani et al. 2003). In fact, the homogeneous and isotropic solutions of the field equations, the FLRW solutions of gravity (Friedman 1922, 1924; Lemaître 1931; H. P. Robertson 1935, 1936a,b; Walker 1937), have not only convinced by their simplicity but also provide a model of the Universe that is in astonishing agreement with observational data (despite a number of open puzzles to which we will come in the following), see sections 2.2 and 2.3. Probably due to the simplicity of these equations, the recording of cosmological data has experienced a substantial upswing during the last decades.

In fact, the today's measurement technology permits to register electromagnetic radiation from astronomical objects that are up to 32 billion light–years away from us (Oesch et al. 2016), and hence, provide information about the Universe from about 13.4 billion years ago. The LIGO and Virgo collaborations have recently succeeded in detecting gravitational radiation from distances of more than 8 billion light–years (B. P. Abbott et al. 2019). The cosmic microwave background (CMB) radiation offers an even more ancient relic of cosmic history (Aghanim et al. 2020a; Penzias and Wilson 1965). It shows a picture of the Universe from the time of decoupling, i.e., from around 13.7 billion years ago (Alpher and Herman 1948c; Peebles, Schramm, et al. 1991). Most of the data points to a very simple picture of the Universe modeled by only six parameters (Aghanim et al. 2020a; Spergel 2014). The corresponding theory is known as the standard inflationary ΛCDM model. A thorough introduction to the current cosmological standard model

will be given in section 2.2. According to this model, the almost homogeneous and isotropic Universe has been expanding over its entire history from a very hot and dense state into the present Universe, presumably starting with a phase of inflationary expansion. The underlying "inflaton" scalar field eventually decayed into other matter species (Albrecht and Steinhardt 1982; Linde 1982) giving rise to the rich cosmic inventory we observe today.

In order to account for the matter content of the Universe, namely the large scale structure of galaxies and the flucutations in the CMB, it is however necessary to introduce *inhomogeneous* cosmological fields (Dodelson and Schmidt 2021; Halliwell and Hawking 1987). In fact, the concordance model of cosmology assumes that small quantum perturbations of the inflaton field provide the seeds of the present large scale structure of the Universe, and induced the necessary inhomogeneities in the early Universe (Bardeen, Steinhardt, and Turner 1983; Guth and Pi 1982; Hawking 1982; Starobinsky 1982). These inhomogeneities are modeled as small Gaussian perturbations (Aghanim et al. 2020a) around the symmetry–reduced model at earliest times, and are stretched to cosmic scales by the continual expansion of space (Blumenthal et al. 1984). For the main part of the known cosmic history, they can be described by classical means but as we go backwards in time, quantum effects should be considered (Baumann 2012). The question of the quantum–to–classical transition of these perturbations has for example been investigated by Kiefer, Polarski, and Starobinsky (1998) and Polarski and Starobinsky (1996), and we will not say much about it here. The purely quantum theoretical part will be discussed in the next paragraph but we remain with the classical late time Universe for the time being.

1.1.3. Problems of the Concordance Model

At the classical level, the above–described procedure of strictly splitting the cosmological fields into a symmetry–reduced part and perturbations thereof provides of course a first mean to study solutions to such a simple model (in contrast to the highly non–linear full Einstein equations) but it leads to several problems and might oversimplify the model at hand: First, at the technical level, it breaks the covariance of the theory, and depending on the concrete problem, it is usually advisable to use a gauge–invariant perturbation formalism (Bardeen 1980; Kodama and Sasaki 1984; Mukhanov, Feldman, and Brandenberger 1992). This might be mathematically cumbersome but does not alter the physical results at the classical level, and provides us indeed with a sound theory of cosmological perturbations. Another problem is however more severe (Abramo, Brandenberger, and Mukhanov 1997): In fact, the procedure for examining the cosmological dynamics starts by solving the purely homogeneous and isotropic, zeroth order contributions to the field equations *independently* of the perturbations. Then, by employing this classical "fixed" background solution in the first order equations of motion for the perturbations and truncating any higher order contributions, one can evolve the cosmological perturbations on this fixed geometry. Due to the split, the background is considered completely independent of the perturbations and thus, possible backreactions of the dynamical perturbations on the homogeneous degrees of freedom are neglected. It is still unclear whether and to which extent these classical backreactions have an impact on the global evolution of the Universe, and we dedicate chapter 3 to an overview of the most relevant results in this field.

One motivation for studying backreaction actually came from the hope that such effects

could shed light on any of the existing discrepancies between the cosmological standard model and observational data (see for example (Buchert 2008)). Some of these hypotheses did not stand the test of numerical studies (Adamek, Clarkson, et al. 2019; Macpherson, Price, and Lasky 2019), others are not tested yet. In any case, it is timely to approach the severe problems of the cosmological standard model and to search for viable solutions for the dark energy and dark matter problems (Bertone and Hooper 2018; Perlmutter et al. 1999; Riess et al. 1998). We also point to the recently discovered discrepancy between different measurement results for the Hubble parameter H_0 (Pesce et al. 2020), and we will be more explicit regarding the open problems of the concordance model in section 2.3. As of today, there exists a variety of proposed solutions among which classical backraction but there is no general agreement on any particular solution. Some approaches suspect to find their answers in earlier phases of the cosmic history. In fact, the above discrepancies in the recent measurements of H_0 could point to inconsistencies of the cosmological concordance model applied to the early Universe (Aghanim et al. 2020b). This brings us to the second important thematic field in physics of the last two centuries – quantum theory.

1.1.4. The Beginnings of Quantum Mechanics

While the revolutionary thoughts on gravity were inspired by the rather well–tried theories of gravitation and electromagnetism by Newton and Maxwell, very novel ideas were needed to describe experimental results at the microscopic scale. Planck (1900a) was the first to find a correct law for the black body radiation by assuming that a cavity wall viewed as a collection of oscillators absorbs and emits radiation only in discrete "quanta" (Weinberg 2015). Shortly after, Einstein (1905a) succeeded in explaining the photoelectric effect (Lenard 1902) also by means of discrete energy quanta of the radiation field. Furthermore, Bohr (1913) with his atomic model of discrete energy levels as well as De Broglie (1923) with his wave–particle dualism contributed to the search for a thorough new theory of "quantum mechanics" (Born 1924; Weinberg 2015). Its theoretical foundations were laid by Born, Heisenberg, and P. Jordan (1926), Born and P. Jordan (1925), and Heisenberg (1925) using a matrix approach, by Schrödinger (1926a,b,c,d) with a wave mechanics formulation, and Schrödinger (1926e) finally established the equivalence of these two approaches (Weinberg 2015). Neumann (1932a) finally succeeded in integrating both theories into a coherent mathematical picture of operator algebras and Hilbert spaces (O'Connor and E. F. Robertson 1996).

The new quantum theory was however incompatible with Einstein's special and general relativity which motivated researchers to find, as a first step, a Lorentz invariant theory of quantum fields, i.e., a theory that incorporates the principles of *special* relativity (Kuhlmann 2020). Born, Heisenberg, and P. Jordan (1926) had already considered the (free) electromagnetic field as an infinite number of quantum oscillators and Dirac (1927) added an interaction term in order to account for the emission and absorption of radiation in a first order perturbative manner (Weinberg 1977). In order to describe electromagnetically interacting matter particles in a Lorentz invariant way, Dirac (1928) established the one–particle equation for electrons and positrons named after him. Accordingly, while radiation was treated in a field formalism, matter particles were understood as individually occurring objects, see the historical overview by Weinberg (1977). P. Jordan and Wigner (1928) showed that material particles can also be regarded as the quanta of fields (e.g.,

the Dirac field) and the idea of a field–theoretical quantum electrodynamics began to take root. The idea was developed further by Heisenberg and Pauli (1929, 1930) and P. Jordan and Pauli (1928), and by Pauli and Weisskopf (1934) and Weisskopf (1934). Furry and Oppenheimer (1934) succeeded to show that quantum electrodynamics naturally incorporates antiparticles which had already been predicted by Dirac (1928), (Weinberg 1977).

The benefits of this quantum theory have been demonstrated experimentally, for example by the correct prediction of additional quantum mechanical degrees of freedom such as electron spin (Debye 1916; Sommerfeld 1916; Uhlenbeck and Goudsmit 1925), and the correct theoretical determination of the fine structure of atomic spectra (Michelson and Morley 1887; Sommerfeld 1940). However, the resounding success of the theory was limited to simple dynamical problems, and in order to describe quantum mechanical interactions, approximation methods had to be used for both relativistic and non–relativistic phenomena. One particularly important approximation method for non–relativistic problems that is still of great relevance today was introduced by Born and Oppenheimer (1927). It introduces the ratio of the small electron mass and the nuclear mass as an "adiabatic" perturbation parameter to establish a first order perturbative theory for molecular systems. The scheme is widely used in theoretical and computational chemistry (Cramer 2004). Despite its success, the Born–Oppenheimer theory is restricted to a narrow class of Hamiltonian systems and cannot be extended to higher perturbative orders. We will be more explicit regarding the Born–Oppenheimer formalism in section 6.1 as it forms the physical basis of this work. A possible extension was introduced by Panati, Spohn, and Teufel (2003), the so–called space adiabatic perturbation theory (SAPT) which overcomes the afore–mentioned shortcomings, see sections 6.2 – 6.8. It requires to introduce a phase space quantization scheme (Groenewold 1946; Moyal 1949; Weyl 1927; Wigner 1932), and pseudodifferential calculus (Hörmander 1979, 1985b; Kohn and Nirenberg 1965).

1.1.5. Perturbative Quantum Field Theory

Perturbative methods to quantum theory have also been employed on the (special) relativistic quantum field theory (QFT) side. In fact, the above–mentioned first models in QFT are *perturbative* in nature (as are most of the theories studied today), and most importantly for us, they rely on a *non–dynamical Minkowski background* (Strocchi 2013). The motivation for developing such perturbative models obviously lies in the complexity of the non–perturbative interacting theories. In fact, we only know a very limited number of QFTs that can be solved exactly, in particular in four space time dimensions these are exclusively the free field theories of any mass and spin, and theories with solutions that can be expressed as functions of such free fields (Strocchi 2013). We will provide a short review of QFT in section 4.1 focussed on the QFT of a free Klein–Gordon scalar field.

Strictly speaking, of course, there is not one single QFT because as numerous as the problems for formulating a quantum theory of physical interactions are, so are the approaches to solving them (Kuhlmann 2020). Streater and Wightman (1964) succeeded to find a mathematically rigorous formulation for these free theories by introducing their Wightman axioms (Strocchi 2013). Unfortunately, none of the known interacting quantum field models in four space time dimensions could be rigorously constructed and thus could be verified to obey these axioms. Now, one

can either try to obtain physically relevant results from these interacting theories, despite the lack of a mathematical foundation, or one can pursue the goal of developing QFTs that satisfy the axioms. In the first case, it is necessary to resort to perturbative methods as had already been recognized by Dirac and his peers. These perturbative approaches assume that the Hamilton operator $\boldsymbol{H}$ of the interacting theory splits into a free solvable Hamiltonian $\boldsymbol{H}_0$ and an interaction term $\boldsymbol{V}$, and that the interaction term enters with a small coupling or perturbation parameter δ such that $\boldsymbol{H} = \boldsymbol{H}_0 + \delta \boldsymbol{V}$ (Kuhlmann 2020): The calculation of scattering amplitudes, i.e., of the S–matrix elements $S_{\alpha,\beta} := \lim_{\tau\to\infty}\langle\alpha, \boldsymbol{U}(t_{-\tau} - t_\tau)\beta\rangle$ requires the (vacuum) states $\alpha, \beta \in \mathcal{H}_0$ in the free Hilbert space $\mathcal{H}_0$ of the free theory and the time evolution operator $U(t_{\text{fi}} - t_{\text{in}})$ evaluated for some initial and final times t_{in}, t_{fi} in the infinite past and future. The time evolution operator in perturbation theory consists of a power series in δ whose coefficents are the time–ordered products of $\boldsymbol{V}$ represented in terms of the free operators. Every perturbative order results in a number of cross sections which represent different particle processes.

Now there are several fundamental problems with these calculations. The first is that the individual scattering amplitudes give infinite results as Oppenheimer (1930) realized in the framework of quantum electrodynamics and these are due to the self–energy of the fields and vacuum polarization. The theory consequently looses its predictive power and many physicists believed back then that the framework was useless. From 1947 on however, QFT experienced a remarkable upswing, triggered by the measurement of an effect of the self–energy of the electron in the hydrogen atom, namely the Lamb shift (Lamb and Retherford 1947), (Weinberg 1977): The year before, Tomonaga (1946), and then in the following years, Tomonaga et. al. (Ito, Koba, and Tomonaga 1948; Kanesawa and Tomonaga 1948; Koba, Tati, and Tomonaga 1947; Koba and Tomonaga 1948; Tomonaga 1946) as well as Schwinger (1948, 1949a,b, 1951a,b) and Feynman (1948a,b,c, 1949a,b, 1950) developed renormalization formalisms which absorb the infinities into a redefinition of the physical parameters (Weisskopf 1936). Dyson (1949a,b) showed that these procedures apply well to quantum electrodynamics but in general only to a very limited number of theories.

Fortunately, through the work by many physicists from the 1950's to the 1970's ('t Hooft and Veltman 1972; Englert and Brout 1964; Fritzsch, Gell-Mann, and Leutwyler 1973; Glashow 1961; Gross and Wilczek 1973; Guralnik, Hagen, and Kibble 1964; Higgs 1964; Politzer 1973; Salam 1968; Weinberg 1974a,b; Yang and Mills 1954), it was possible to formulate a certain class of physically relevant theories which are indeed renormalizable (Weinberg 1977): These are the gauge theories for the interactions subsumed in the Standard Model of physics: The electroweak interactions as well as the strong interaction together with the Higgs mechanism of spontaneous symmetry breaking. Within these theories, it is possible to compute finite values for the scattering amplitudes which are in astonishing agreement with experimental data. We refer to the discovery of the zoo of Standard Model particles, and especially to the detection of the Higgs boson at the LHC (Aad et al. 2012; Chatrchyan et al. 2012).

Despite the experimental agreement, the Standard Model stands on rather thin mathematical grounds as we have explained above. Besides, an important result which questions the construction of a perturbative QFT using the tools of the free theory was formulated by Haag (1955). Namely, the free and the fully interacting Hamiltonian give rise to different unitarily inequivalent representations (D. Hall and Wightman 1957). It turns out that this also applies to free neutral scalar fields of different mass and hence, prevents these models from having unitarily equivalent

representations (Reed and Simon 1975b). We will encounter similar problems in the construction of the cosmological QFT in this thesis (see sections 8.1 and 9.1) which can however be (partially) circumvented by introducing a suitable set of transformations for the fields.

1.1.6. Quantum Field Theory on Curved Space Times

So far, we restricted our considerations to perturbative models of QFT which heavily rely on a static Minkowski background. In fact, standard Minkowski QFT only admits the matter fields as dynamical entities while treating space time as static. This kind of simplification is of course reasonable as long as space time is almost Minkowskian, for example for Earth–based particle experiments but for the cosmological situations that we have in mind we need to drop this assumption. One can anticipate that such an endeavor will aggravate the theoretical problems of perturbative QFT substantially but there are several proposals for how to make progress, and we will present them in the following. To start with let us point out that so far, the matter fields are considered in a quantum framework while the metric field is considered classically. However, Einstein's equations directly relate the quantum matter content with the classical space time geometry which appears to be a contradiction from a mathematical perspective. Although not providing an answer to the question of why we should treat quantum fields and a classical geometry at the same level, QFT on CSTs try to provide a connection between standard Minkowski QFT and general relativity.

The idea of QFT on generically curved space times (Fulling 1989; Hollands and Wald 2010; Wald 1995) is to consider classes of classical geometries and to examine the QFTs given such geometries. This is of course not a trivial enterprise since standard QFT heavily relies on the notion of a preferred vacuum state and an associated Hilbert space of excited particles. The existence and uniqueness of such a preferred vacuum is due to the strong Poincaré symmetry of Minkowski space, and hence completely looses its relevance on generically curved space times. A framework that does not rely on representations of the quantum theory but which focusses on the operator algebraic aspects, and which is hence much more flexible when it comes to generic space times is algebraic QFT (Araki 1999; Brunetti, Dappiaggi, et al. 2015; Haag 1955). Chapter 4 is devoted to several aspects of QFT on CST, and section 4.1 particularly introduces and discusses the algebraic approach.

However, such theories obviously make an important simplification: Similar to the backreaction problem in classical cosmological perturbation theory, they omit the effects of one part of the system (here, of the quantum matter fields) on another part (the geometry of space time). This cuts out a relevant part of the interactions within the system. While it is certainly a progress to consider the geometry of space time as a dynamical entity, one only examines the propagation of the quantum fields on the latter while neglecting their effects on the space time geometry. There are several proposals for how to include such backreaction effects, namely semiclassical gravity (Ford 2005; Wald 1977), and stochastic (semiclassical) gravity (Calzetta and Hu 1987; Hu 1989; R. Jordan 1986, 1987). Both approaches will be discussed in sections 4.2 and 4.3 respectively, and we provide the reader with an overview of the current state of research in these fields.

Although these approaches provide the possibility of including backreaction effects at a semiclassical level, the fundamental issue of equating a classical with a quantum mechanical en-

tity via Einstein's field equations remains unanswered. This suggests in fact to rethink the methods used so far, and it seems natural from the previous discussion to consider the gravitational field as a quantum mechanical field. As a first step in formulating such a theory of quantum gravity, one could consider a perturbative framework in which the gravitational perturbations of a Minkowski metric (i.e., gravitons) are being quantized in the same manner as the quantum matter fields of standard QFT and using the same Fock representations. As it turns out, such perturbative theories are non–renormalizable ('t Hooft and Veltman 1974; Goroff and Sagnotti 1986), and which should prevent the whole endeavor right from the beginning. One could now argue that it is still possible to formulate an effective field theory for low energies as proposed by Donoghue (1994). In order to describe situations with high energy densities as we have in mind, this is however of little utility.

1.1.7. Quantum Gravity and its Open Problems

We are hence led to consider fully *non–perturbative* approaches to quantum gravity. The formulation of such a non–perturbative theory of quantum gravity has occupied researchers for over a hundred years now, in particular since Einstein (1916b) first speculated about the modifications that quantum theory would bring for general relativity (Rocci 2013). At present, we have a number of different approaches for quantizing gravity, among which asymptotic safety (Niedermaier and Reuter 2006; Weinberg 1976, 1980), string theory, in particular in its AdS/CFT–incarnation (Ammon and Erdmenger 2015; Polchinski 2005), causal dynamical triangulations (Ambjorn, Jurkiewicz, and Loll 2005; Loll 2020), causal sets (Bombelli et al. 1987; Sorkin 2003) as well as spin foam and loop quantum gravity (LQG) (Rovelli 2010; Thiemann 2008) to mention but a few. We emphasize that remarkable progress has been made in the theoretical and phenomenological elaboration of these theories during the last years. Unfortunately, none of them has so far been able to provide a uniform model for describing the cosmological data situation, and the mathematical formulation of any of these theories of quantum gravity is a highly complex endeavor.

We refer exemplarily to LQG which provides a mathematically sound framework to formulating the quantum dynamics of gravity including a rigorous representation of the canonical commutation relations and in which even the problem of gauge reduction can be solved using material reference systems (Giesel and Thiemann 2015; Thiemann 2008). The problem in this particular quantum gravity framework is then related to the fact that the quantum dynamics is plagued by quantization ambiguities which have found their way into the quantum Einstein equations after removing an auxiliary regulator. This problem is more precisely due to the tremendous non–linearity of the Einstein equations, and hence prevents the prediction of testable results. Since however LQG is a *non–perturbative* approach to quantum gravity, at least no perturbation series have to be summed with unknown (presumably zero) radius of convergence. To make LQG predictive, many efforts are made regarding non–perturbative (Wilsonian) renormalization for LQG, for example by Bahr (2017), Bahr and Steinhaus (2017), Dittrich (2017), Dittrich and Steinhaus (2014), Lang, Liegener, and Thiemann (2018a,b,c,d), and Liegener and Thiemann (2020).

In addition to the open questions on the theoretical side, one major problem in the development of a theory of quantum gravity is the lack of relevant measurement data owing to the fact that the large reduced Planck mass $M_{\mathrm{Pl}} = \sqrt{\hbar c/(8\pi G)} \approx 4.34 \times 10^{-9}$ kg $\approx 2.43 \times 10^{18}\mathrm{GeV/c^2}$

(NIST–Database 2019) suppresses any quantum gravity effects in earth based experiments. In fact, the heaviest known Standard Model particle (or rather boson) is the Higgs with a mass $M_{\mathrm{H}} \approx 125.10\mathrm{GeV/c}^2 \ll M_{\mathrm{Pl}}$ (Zyla et al. 2020). The huge mass difference is known as the hierarchy problem. On the other hand, this specifically allows to develop perturbation theories for gravitational models coupled to matter. This will be particularly important for our purposes here as we are going to introduce a perturbative scheme with respect to ${M_{\mathrm{Pl}}}^{-1}$, or rather its ratio with a typical Standard Model coupling constant. In fact, the idea to use ${M_{\mathrm{Pl}}}^{-1}$ as a perturbative parameter in quantum gravity or cosmology has a long tradition and goes back to Brout (1987), (Kiefer 2007). We will provide an overview of its applications to quantum gravity and cosmology in chapter 5.

While this large mass difference prohibits to test quantum gravity effects on Earth, there is hope that the increasing abundance of cosmological data can improve the situation. In order to make contact between empirical data and a fully–fledged theory of quantum gravity, one would, in a first place, seek the cosmological sector of such a theory by examining specific states in the physical Hilbert space which possess the appropriate semiclassical "cosmological" properties. Unfortunately, none of the existing approaches has yet reached a stage where such (exact) solutions are available, in particular when gravity additionally couples to matter. This is however indispensable in order to bridge the gap between theory and experiment. More precisely, only if such a semiclassical regime of the theory exists, it will be possible to identify a viable candidate theory of quantum gravity. Due to the non–linear character of the resulting field equations, the intricate coupling between matter and gravity as well as the inherent problems of any quantization procedure for an infinite number of degrees of freedom, any effort to extract exact solutions of a quantum gravity–matter system (even when restricted to cosmological situations) appears to be pointless at present.

1.1.8. Born–Oppenheimer for Quantum Gravity and Semiclassical Limit

Fortunately, the situation is not hopeless and we can anticipate to make progress by considering suitable approximation schemes. Unsurprisingly, the tiny inverse Planck mass can now be of considerable advantage – its occurence in the quantum Einstein equations can serve to establish a rigorous perturbation scheme. From a physical point of view, such a scheme would probably divide the system, at least formally, into a matter and a gravitational part, since the inverse mass values of the Standard Model matter fields are significantly larger than ${M_{\mathrm{Pl}}}^{-1}$. This picture alludes to the idea of an "adiabatic" limit in which the gravity part appears as the zeroth order subsystem while the quantum matter content is associated with a perturbative subsystem that *backreacts* on the gravitational degrees of freedom. Recall therefore the well–known ideas of the Born–Oppenheimer approximation. Such a perturbation theory might not only help to extract viable results from the quantum theory itself but could serve to establish the semiclassical limit of quantum gravity.

Our observations teach us that this semiclassical limit should yield a QFT on CST, similar to what the ΛCDM model refers to during the earlier stages of the Universe. Hence, in this limit the theory describes gravity in (almost) classical terms while the matter content features entirely quantum mechanical characteristics. Consequently, the approximation scheme naturally splits

the system into a gravity and a matter part. Indeed, it turns out that the first approximation scheme with respect to the inverse Planck mass, and the semiclassical limit are intimitely related – but it is important to stress that they are not equivalent. In fact, it is possible to consider the ${M_{\mathrm{Pl}}}^{-1}$–limit without making reference to a semiclassical limit at all as we will explain in a moment. However, both approaches naturally include a split between matter and gravitational degrees of freedom which could allow us to formally separate the problems in order to make progress.

This is why many researchers have considered the ${M_{\mathrm{Pl}}}^{-1}$–limit in order to make progress regarding the semiclassical limit, and which is a perfectly legitimate proceeding. In many approaches, regardless of the underlying quantum gravity formalism, the semiclassical limit is then invoked in a second step by defining suitable semiclassical, maybe coherent, quantum states which have low fluctuations around a given classical metric. Before amounting to the difficulties related to defining such semiclassical states, let us shortly specify the ideas that have been pursued regarding the ${M_{\mathrm{Pl}}}^{-1}$– and the semiclassical limit in quantum gravity. Many of them but not all refer to the Born–Oppenheimer approximation or extensions thereof.

The first investigations using an ${M_{\mathrm{Pl}}}^{-1}$–expansion within quantum gravity–matter models were performed in the framework of quantum geometrodynamics (Kiefer 2007; Wheeler 1957) by expanding the Wheeler–DeWitt equation in terms of the ratio of the Planck mass and the matter field mass (Kiefer and T. P. Singh 1991), and possibly by using the Born–Oppenheimer approach (Bertoni, Finelli, and Venturi 1996; Brout and Venturi 1989; Kiefer 1994) (for a summary, see (Kiefer 2007)). In a second step, these approaches employ the typical Born–Oppenheimer ansatz solution that seperates the system into a gravitational and a matter part (Kamenshchik, Tronconi, and Venturi 2020; Kiefer 2007). Integrating out the matter part gives rise to an effective quantum problem for the geometric part including the backreaction effects of the quantum matter system. Note that there is no semiclassical limit invoked so far. However, in a second step, one can additionally employ a semiclassical approximation giving rise to a matter QFT on CST. In this respect, it is common to employ a Wentzel–Kramers–Brillouin (WKB) ansatz (Brillouin 1926; Kramers 1926; Wentzel 1926), for the geometrical states, yielding a set of semiclassical Einstein equations. Such states are however not coherent and do not solve the quantum constraint. In this respect, the question of time and of unitary evolution arises, and we refer to the book by Kiefer (2007) and the more recent paper by Di Gioia et al. (2021) and references therein for a discussion of this topic. We will be more precise regarding these approaches (and others) within the geometrodynamical paradigm that attempt to better incorporate interactions between the gravity–matter components in chapter 5.

Other attempts to implement the Born–Oppenheimer approximation in quantum gravity–matter systems have been pursued by Giesel, Tambornino, and Thiemann (2009) in an LQG–related framework. While the Born–Oppenheimer approximation represents an ideal framework for including backreactions, its applicability is quite restrictive. In fact, the choice of variables within LQG prevents the direct use of the Born–Oppenheimer methods as the flux operators are mutually non–commuting (which is a prerequisite for the Born–Oppenheimer scheme). Consequently, the authors use another set of variables for the gravity sector and a scalar field for the matter sector to derive a set of semiclassical Einstein equations. They also point to the possibility of pursuing the formal Born–Oppenheimer scheme and computing *quantum* solutions to the gravity sector with the effective backreaction of the quantum matter fields, and propose to introduce

coherent states for the gravitational subsystem in order to make progress in finding solutions.

Unfortunately, the construction of such semiclassical, coherent states within a full theory of quantum gravity is a highly non–trivial task. In LQG, for example, candidates for such coherent states have been extensively studied by Thiemann (2001) and Thiemann and Winkler (2001a,b,c). Nevertheless, the task of defining the semiclassical limit within LQG and within other approaches to quantum gravity by means of such states could not be fully addressed, and it is, in general, a difficult exercise, see for example in (Sahlmann and Thiemann 2006a,b; Stottmeister and Thiemann 2016a,b,c) for works within LQG. More precisely, these coherent states are primarily defined for a free gravitational system, and fail to follow the classical trajectory in interacting systems with matter for a sufficiently long time, i.e., the quantum Hamiltonian does not preserve their semiclassical properties. The difficulty of defining such states for full quantum gravity plus matter has motivated several lines of research in order to make progress regarding the semiclassical limit, and which has also stimulated research for understanding the (more generic) problem of quantum backreaction in such models.

One idea is of course, again, to recover first a formal split between quantum gravity and matter degrees of freedom, and which would facilitate the implementation of the semiclassical limit and the possible quest for suitable semiclassical states. In this respect, Stottmeister and Thiemann (2016a,b,c) considered the application of the SAPT scheme within LQG. While the application of this scheme allows to consider the question of pure quantum backreaction, it is also ideally suited to investigate the semiclassical limit due to the reasons mentioned above. Since in the SAPT approach, the variables of the gravitational (adiabatic) sector are not required to commute, it is in principle possible to apply the Born–Oppenheimer ideas also to LQG and related theories, which was not possible before (see above). The concrete implementation turns however out to be difficult due to the particular structure of the LQG phase space and its quantum representation, see chapter 5 for more details.

1.1.9. Making Progress with Symmetry Reduction

All these difficulties regarding the question of backreaction in full quantum gravity and the derivation of the semiclassical limit suggest to first consider simpler, possibly symmetry–reduced models of quantum gravity with matter. I.e., like in many other situations, it seems reasonable to first explore symmetry reduced models before attacking the less symmetric situations – connected with the hope of obtaining at least qualitative statements. These so–called "minisuperspace" models perform first a symmetry reduction in the classical theory and then quantize the finitely many, remaining degrees of freedom. Of course, this procedure stands in opposition to Heisenberg's uncertainty principle which prohibits the freezing of what are actually quantum mechanical, fluctuating degrees of freedom. While Kuchar and Ryan (1989) have shown that some symmetry reduced models do not reflect the behavior of less symmetric models in metric gravity, there is no generic result that prevents the symmetry reduced models from serving as an arena for testing mathematical methods. In line with the various approaches to quantum gravity, there is a multitude of attempts to define a quantum cosmology, e.g., the canonical Wheeler–DeWitt approach (DeWitt 1967), the standard path integral approach due to Hartle and Hawking (Hartle and Hawking 1987; Hawking 1987), string cosmology (Veneziano 1991), spinfoam cosmology (Vidotto 2011),

and canonical loop quantum cosmology (LQC) (Ashtekar, Bojowald, and Lewandowski 2003a; Ashtekar, Pawlowski, and P. Singh 2006b; Bojowald 2008) and many more.

To approach our goal of describing the interactions of full quantum gravity plus matter, it is of course indispensable to include inhomogeneities in such models. In a first step, this might be done using linear perturbation theory for simplifying our enterprise and also in recognition of cosmological observations. Such approaches hence include dynamical cosmological perturbations as well as a dynamical homogeneous sector. Thus, they still fall into the category of *non–perturbative approaches to quantum gravity* in comparison to the traditional perturbative Minkowski space plus graviton frameworks, and should consequently be ideally suited to describe the interactions within the very early Universe. At the same time, they might alleviate the problems associated with the substantial non–linearities in Einstein's field equations. Similar to the full theory, however, these models pose a number of question if one aims at understanding and describing the interactions of the components or derive a semiclassical limit.

Progress with respect to the semiclassical limit can be achieved by computing expectation values with respect to some admissible semiclassical ansatz state. Most easily, one starts with considering semiclassical states for the homogeneous quantum degrees of freedom but of course it is (in principle) possible to extend the procedure to the quantum perturbations. To start with, one may derive a semiclassical trajectory of the homogeneous degrees of freedom using such semiclassical states for the homogeneous sector, giving rise to a formal QFT on CST. The latter now includes effective quantum modifications to the semiclassical homogeneous curved space time. The additional (gauge–invariant) cosmological perturbations on this effective background are then quantized using standard Fock representations. As examples, we point to the hybrid quantization schemes in LQC (i.e., the dressed metric approach (Agullo, Ashtekar, and Nelson 2012), the deformed algebra approach (Barrau et al. 2015) and the hybrid approach (Elizaga Navascués, Martin-Benito, and Mena Marugan 2016; Martín–Benito, Garay, and Mena Marugan 2008)) which use different methods to establish effective quantum field equations of motion for the cosmological perturbations on an LQC effective quantum background.

Common to these approaches is that they choose a specific product ansatz for the wave function with a homogeneous and an inhomogeneous contribution, in close analogy to the standard Born–Oppenheimer ansatz. They determine effective equations of motion for the quantum perturbations on an effective semiclassical homogeneous quantum background which hence corresponds to a QFT on CST with a modified cosmological space time. On the other hand, they neglect backreactions in the sense of a Born–Oppenheimer approximation from the perturbations on these approximate homogeneous solutions, and are consequently unable to provide a better understanding of the interactions within the quantum gravity–matter system. The assumptions that went into these approaches and which are in our opinion not easy to control have been detailed by Castelló Gomar, Martín-Benito, and Mena Marugán (2015) for the hybrid and by Agullo, Ashtekar, and Nelson (2013) for the dressed metric approach.

Moreover, these approaches rely on introducing one specific semiclassical state. To (partially) overcome these shortcomings, considerations of including backreaction have been pursued by (Rovelli and Vidotto 2008) and by Castelló Gomar, Martín–Benito, and Mena Marugán (2016) within the LQC approach, and by Chataignier and Krämer (2021) and references therein within the geometrodynamical approach. Many of these approaches remain however on a purely formal

level due to technical difficulties or rely on a set of specific semiclassical ansatz functions.

1.1.10. Space Adiabatic Perturbation Theory in Quantum Cosmology

It is precisely at this point that we propose a new but at the same time conservative formalism to describe the interactions within a non–perturbative theory of quantum gravity plus matter, and which improves the current state of the art in several respects. More specifically, we implement a perturbative approach with respect to the inverse Planck mass that is able to rigorously attack the question of whether the backreactions of the inhomogeneous cosmological quantum fields have a substantial effect on the homogeneous quantum degrees of freedom – A very crucial open problem that has been neglected in most approaches so far (mostly due to technical problems), and which represents the first important step towards a thorough understanding of the interactions in quantum gravity–matter systems, and a step towards a semiclassical limit of the theory.

As opposed to the approaches above, we will not rely on the introduction of some semiclassical ansatz functions for the homogeneous sector. We are hence, for the time being, not primarily interested in the semiclassical limit of the respective models but rather in formulating a consistent approach for obtaining effective and simpler constraints or equations of motions that take the full quantum mechanical and dynamical character of non–perturbative quantum gravity into account. Of course, it is still possible to consider the semiclassical limit in a second step. As anticipated above, our goal is to develop and implement a perturbative scheme following the ideas of the Born–Oppenheimer approach but which improves the latter in several essential ways. The space adiabatic approach by Panati, Spohn, and Teufel (2003) represents an ideal starting point for achieving just this. Their original formalism will be presented in chapter 6.

Its Advantages

The considerable advantages of employing SAPT methods in order to approach a working theory of interactions in quantum cosmology plus matter can be identified by comparing to the above mentioned approaches: First, while adhering to the sucessful idea of considering an ${M_{\mathrm{Pl}}}^{-1}$–limit in quantum gravity, it establishes a rigorous perturbative formalism with respect to ${M_{\mathrm{Pl}}}^{-1}$ which can be evaluated up to any desired order. This allows to derive effective quantum Hamilton constraints or operators whose structure is much simpler than the original one but whose solutions approximate the true solutions up to an, in principle, indefinitely small error. Secondly, these technically much simpler constraints are derived without invoking a semiclassical limit or behaviour of any kind. We are also not forced into choosing one specific (semiclassical) ansatz state in order to derive physical results as it is required by most of the approaches considered before. Thirdly, the scheme performs a formal split between the homogeneous and the inhomogeneous sector in quantum cosmological perturbation theory, and which allows to analyze the two subsystems (again on a formal level) at different stages of the procedure. This split brings us one step closer to recovering the semiclasssical QFT on CST–limit of quantum cosmology, and might simplify the identification of suitable semiclassical states considerably. Finally, since the formalism relies on a phase space quantization scheme, it substantially enlarges the range of systems to which it can be applied – most importantly, to the cosmological systems that we have in mind. Recall that the

Born–Oppenheimer approach restricts to models in which the coupling of subsystems is mediated via commuting operators. SAPT lifts this restriction, and makes it hence possible to apply such a scheme at all.

Our Achievements

With these prerequisites in mind, we have hence achieved the following goals on the way to a rigorous formulation of a theory of interactions in coupled quantum gravity plus matter:

- We have shown that the methods of SAPT as introduced by Panati, Spohn, and Teufel (2003) for *unconstrained*, quantum mechanical systems can be extended to *constrained* Hamiltonian systems, most importantly to problems in quantum cosmology. In fact, the constraint itself thereby justifies the use of the perturbative (adiabatic) hierarchy rather than the equipartition theorem. This will be made very clear in chapter 7 where we introduce a cosmological toy model in order to test the application of SAPT to constrained systems. More precisely, we apply the scheme up to second (adiabatic) order to a homogeneous and isotropic FLRW model with a scalar field as the matter content.
- SAPT also applies to quantum field theoretical models. In fact, we show that a general obstruction to implementing the SAPT formalism to such infinite dimensional theories is the failure of the Hilbert–Schmidt condition. This generically indicates that the dynamics of the quantum cosmological perturbations in such theories is not unitarily implementable. In chapter 8, we examine this problem for a cosmological model with scalar matter field perturbations and propose a transformation of variables which alleviates the failing of the Hilbert–Schmidt condition. We then successfully apply SAPT to cosmological perturbation theory with a scalar field and dust matter content up to second order in the adiabatic perturbations. This results in an effective Hamilton operator for the homogeneous sector and which takes the backreaction of the perturbations thoroughly into account.
- We are able to identify an important challenge which occurs when implementing SAPT to quantum cosmological perturbation theory: The transformations of variables mentioned before yield modified mass values or rather mass functions of the perturbation fields. In particular, the mass squares become functions of the homogeneous variables and may be indefinite, inducing tachyonic instabilities for the perturbations. In chapter 9, we point to a number of solutions to this problem, and apply one of them to the model in chapter 8 and also to the next model considered in chapter 9. We also assert that the standard transformations to gauge–invariant cosmological perturbations already lead to such tachyonic fields, hence the very occurence of such tachyonic instabilities is not first and foremost due to the SAPT scheme.
- We apply SAPT to the standard gauge–invariant cosmological perturbation model in quantum cosmology up to second order in the adiabatic perturbations in chapter 9. Again, the transformations for obtaining gauge–invariant variables and in order to circumvent the Hilbert–Schmidt condition lead to indefinite mass squared functions for the scalar and tensor perturbations. These functions are non–polynomial with respect to the homogeneous degrees of freedom. As mentioned before, we propose several strategies for coping with

these peculiar mass functions, and apply one of them to the cosmological model in this chapter.

- Despite the indefinite mass squared functions, we emphasize that SAPT can always be formally carried out. One simply needs to assure that the tachyonic phase space regions as well as regions where the eigenvalues of the perturbative fields cross are avoided when quantizing the homogeneous sector. One possibility is to restrict the underlying phase space by hand, which is conceivable due to the phase space quantization procedure pursued here.
- For all the cosmological models considered in this thesis, i.e., the purely homogeneous model in chapter 7, the scalar and dust field cosmological model with inhomogeneities in chapter 8, and the perturbative scalar field model with gauge–invariant scalar and tensor perturbations in chapter 9, we are able to compute an effective Hamilton constraint or operator that takes the backreaction of one part of the system onto the remaining system into account. Finding solutions for this considerably simpler Hamiltonian will provide us with approximate solutions to the coupled gravity–matter system, and which takes their interactions adequately into account. While formally symmetric, these effective Hamiltonians are non–polynomial, both in momentum and configuration degrees of freedom, leading to unpleasant domain issues. We emphasize however that such questions of self–adjoint extensions are generic in quantum gravity and not caused by the SAPT scheme itself. We have identified possible choices of dense domains.

This being said, we finally take the opportunity to emphasize once again that our considerations of backreactions are performed in a purely non–perturbative quantum gravity framework, i.e., the inhomogeneous as well as the homogeneous degrees of freedom are both dynamical and quantum. In particular, we do not refer to any background structure like in perturbative Minkoswki quantum gravity. The use of the *cosmological* perturbation series up to linear order is a tool for simplifying the calculations and should not be confused with a perturbative limit of quantum gravity implying a background structure. While the pure quantum gravitational theories have not yet reached a stage in which physical solutions are known, the cosmological split performed in this work permits to make progress in this direction – while still considering *all* degrees of freedom in a quantum framework. Hence, our application of SAPT provides a formidable avenue to better understanding and possibly solving purely non–perturbative quantum cosmological models, thoroughly taking into account the interactions between matter and gravity. Very importantly, due to the natural split of its degrees of freedom and the formal consideration of homogeneous and inhomogeneous degrees of freedom at different levels of the scheme, it offers the attractive perspective to also simplify the quest for a semiclassical limit of quantum cosmology.

We will provide a detailed summary of our findings in part IV and point to the numerous future routes entailed by our work. The next section provides a short and more concise outline of this thesis (i.e., without historical references).

1.2. Outline

Following the thematical map given above, the structure of this thesis is as follows:

In part II, we provide the reader with the necessary mathematical tools and physical background for this thesis. We thereby assume the reader to be familiar with the basic notions of general relativity, the concordance model of cosmology and QFT. In order to make this work as self–contained as possible, we will nevertheless review some of the relevant issues within these fields. We start in chapter 2 with the theory of general relativity and the concordance model of cosmology. We will use the opportunity to point to the various open questions and problems of the contemporary cosmological model. This will subsequently bring us to chapter 3 which reviews the current state of research in the field of classical cosmological backreaction. There, the question is whether and to which extent classical cosmological inhomogeneities in the rather recent Universe might modify the evolution of the Universe on its largest scales. As it turns out, there is no consensus, and opinions about the interpretation of the physical results differ widely.

We then leave the purely classical realm of the cosmic history – going backwards in time – and start in chapter 4 with a short review of QFT on CST. This will prove to be useful for the subsequent sections which discuss the backreaction problem in the semiclassical theory. Here, semiclassical means that matter fields are considered as quantum fields which propagate on a purely classical space time, and thus the question of backreaction is whether those quantum fields alter the classical Einstein equations for gravity. One possible path to examining this question, denoted as semiclassical gravity, computes the expectation value of the quantum stress–energy tensor in a suitable (cosmological) quantum state of the matter fields and uses the result as an effective source for the classical Einstein equations. The second approach that we will discuss is denoted as stochastic (semiclassical) gravity, and adds stochastic noise terms that account for the quantum fluctuations of the matter fields. Both approaches are shortly reviewed and the current state of research is presented.

Further proceeding backwards in time, the concordance model of cosmology suggests that a purely quantum mechanical framework of the physical interactions in the very early Universe should be considered. Accordingly, in chapter 5, we review the notion of backreaction in purely quantum (field) theoretical approaches to gravity. More precisely, we will specifically point to the works in quantum gravity and quantum cosmology that employ the inverse Planck mass as a perturbation parameter to evaluate backreaction similar to the approach that is promoted in this thesis.

This brings us to the final chapter 6 of the introductory part II which is dedicated to the analysis of coupled quantum systems using appropriate approximation schemes. It introduces SAPT as promoted by Panati, Spohn, and Teufel (2003) which will be used for the computation of backreaction in the following chapters. The approach is inspired by the standard Born–Oppenheimer approximation for molecules (which will be reviewed as well) but uses advanced mathematical tools in order to enlarge the scope of the scheme and to provide a systematic perturbation theory. It uses a phase space quantization for parts of the physical system and employs pseudodifferential calculus in various ways. More precisely, it relies on an operator–valued pseudodifferential calculus which will be thoroughly introduced in chapter 6. We will provide a systematic iterative evaluation of the scheme as well as the explicit formulae of this perturbation scheme up to second perturbative order (which are particularly relevant for the remaining chapters). We finish with a showcase example of two coupled oscillators.

In part III, we use and extend SAPT in order to compute the backreaction effects for cosmo-

logical systems. Thereby, we encounter several difficulties since we apply the scheme to quantum field theoretical models while the original theory is conceived for finite–dimensional quantum systems.

As a warm–up, chapter 7 discusses a homogeneous and isotropic cosmological model that consists of the geometric FLRW degrees of freedom (i.e., the scale factor and its conjugate momentum), and a homogeneous and isotropic real scalar field. We compute the backreaction from the scalar field to the geometry. While the evaluation of SAPT proceeds in a very similar way as for the oscillator model, there are new challenges that we will discuss in detail. In fact, due to the constraint character of general relativity, the identification of slow and fast sectors like in the Born–Oppenheimer theory is not trivial, and the special form of the Hamilton constraint induces the occurrence of non–polynomial operators in the final effective Hamilton constraint.

In chapter 8, we apply the ideas of SAPT to a quantum field theoretical model that consists of a homogeneous and isotropic geometry and a dust particle that serves to deparametrize the model (i.e., to introduce a clock) as well as a quantized Klein–Gordon scalar field. Before applying the space adiabatic formalism, it is appropriate to introduce a set of transformations on the whole classical phase space. These transformations will assure that (up to second order in the cosmological perturbations) the QFTs parametrized by the FLRW geometry can be linked unitarily which is a necessary prerequisite for the space adiabatic quantization scheme.

Finally, chapter 9, as the centerpiece of this thesis, examines the backreaction of gauge–invariant cosmological perturbations on a homogeneous and isotropic FLRW model including the homogeneous mode of a real–valued scalar field. It includes an FLRW metric and perturbations thereof as well as a perturbed Klein–Gordon scalar field which are combined in order to define gauge–invariant scalar, vector, and tensor perturbations. As for the previous model, we start by introducing appropriate phase space transformations that are canonical up to second order in the perturbations in order to obtain a well–defined QFT, and in order to allow for a quantization of the total system. We thereby follow the ideas of Castelló Gomar, Martín-Benito, and Mena Marugán (2015) and Martínez and Olmedo (2016). Subsequently, we discuss the presence of indefinite mass squared functions, and possible methods to circumvent the subsequent problems. Finally, we come back to the question of identifying slow and fast sectors and provide some ideas in order to achieve such an identification.

Part IV concludes the thesis by providing a summary of the work and giving an outlook to possible future avenues entailed by our findings. In chapter 12, we provide a detailed summary of this thesis in French in which we recapitulate every chapter seperately.

The appendices A, B and C detail some of the computations that are relevant to the understanding of the thesis but can readily be assigned to the end. In appendix A, we provide computations regarding the Born–Oppenheimer scheme in chapter 6 that help to understand the equations stated there. In appendix B, we detail the computations for the spectral deviations of the anharmonic osillator problem in chapter 6 that are due to the second order backreaction of the harmonic oscillator subsystem. In appendix C, we give a prescription for a Weyl quantization for a system with a compact configuration space.

1.3. List of Publications

This thesis mainly relies on the following publications that resulted from collaborations of the author with T. Thiemann (and one of them also in collaboration with J. Neuser),

i) "Quantum Cosmological Backreactions I: Cosmological Space Adiabatic Perturbation Theory" by Schander and Thiemann (2019a),

ii) "Quantum Cosmological Backreactions II: Purely Homogeneous Quantum Cosmology" by Neuser, Schander, and Thiemann (2019),

iii) "Quantum Cosmological Backreactions III: Deparametrized Quantum Cosmological Perturbation Theory" by Schander and Thiemann (2019b),

iv) "Quantum Cosmological Backreactions IV: Constrained Quantum Cosmologial Perturbation Theory" by Schander and Thiemann (2019c).

As a consequence, parts of this thesis are based or are strongly inspired by these publications. In the relevant chapters, we will point more precisely to the respective publications.

In order to already provide an overview, reference ii) elaborates on the two toy models discussed in section 6.8 and chapter 7, in particular the oscillator model and the homogeneous and isotropic cosmological model. Reference iii) is devoted to the inhomogeneous cosmological model with dust matter that we encounter in chapter 8. Reference iv) examines the inhomogeneous cosmological model with gauge–invariant scalar and tensor perturbations which is the subject of chapter 9. Besides, it provides the precise formulae of the space adiabatic scheme up to second order in the adiabatic perturbations that we give in section 6.7. Finally, reference i) details the conceptual issues encountered when applying SAPT to the (inhomogeneous) cosmological models and which we discuss at various stages of this thesis. Again, a precise statement about the content of the chapter and the corresponding references will be given at the beginning of each chapter.

Further publications that have been published by the author and collaborators during the preparation of the author's thesis are,

v) "Detailed investigation of the duration of inflation in loop quantum cosmology for a Bianchi–I universe with differrent inflaton potentials and initial conditions" by Martineau, Barrau, and Schander (2017),

vi) "Backreaction in Cosmology" by Schander and Thiemann (2021).

Reference vi) is a resume of the application of SAPT to cosmological models and arose during the writing of this thesis manuscript. Certain sections therefore strongly resemble paragraphs of this reference. We will identify these sections in the appropriate places.

Part II.

Research Context and Embedding

2. General Relativity and Concordance Cosmology

In this thesis, we introduce and develop quantum cosmological models that take backreactions from one part of the system on the remaining part into account. In particular, the ultimate goal is to consider gauge–invariant quantum cosmological perturbations and their backreaction on a homogeneous and isotropic quantum FLRW background. Thereby, we build on the pillars of Einstein's theory of general relativity and on (some aspects of) the concordance ΛCDM model of cosmology. In this chapter, we provide the basic ideas and results of these theories with a focus on those notions relevant for our purposes. We assume familarity with the basic concepts of general relativity and the standard cosmological model, and refer the reader to the excellent textbooks by Wald (1984), Carroll (2014), Weinberg (1972), Misner, Thorne, and Wheeler (1973) and Sachs and Wu (1977) regarding general relativity, and by Mukhanov (2005), Dodelson and Schmidt (2021), Durrer (2008) and Baumann (2012) for the concordance model of cosmology. This chapter is based on these references (among others). Some parts of this chapter, especially section 2.3 are inspired and partially taken from reference (Schander and Thiemann 2021) which resulted from a collaboration of the author and T. Thiemann.

Throughout this chapter, we assume $\mathcal{M}$ to be a smooth four–dimensional Lorentzian manifold with signature $(-,+,+,+)$, and we identifiy points X with coordinates thereon. We denote the bundle of (r,s) tensors over $\mathcal{M}$ by $T^r_s\mathcal{M}$, and accordingly the space of sections of $T^r_s\mathcal{M}$ by $\Gamma(T^r_s\mathcal{M})$. Greek indices run from 0 to 3 while latin indices run from 1 to 3. We use units with $c \equiv 1 \equiv \hbar$.

2.1. General Relativity and the ADM Formalism

The theory of general relativity relies on the strong equivalence principle which implies that any theory of gravitation has to be described in terms of a pseudo–Riemannian space time geometry, and the corresponding field equations must admit a certain form (Dittus and Lämmerzahl 2005). More precisely, general relativity ties the geometry of space and time, parametrized by the symmetric two–times covariant metric tensor field $g \in \Gamma(T^0_2\mathcal{M})$, to the (matter) stress–energy tensor field $T \in \Gamma(T^0_2\mathcal{M})$. The relation is provided by Einstein's famous field equations (Wald 1984)

$$G_{\mu\nu} := \mathcal{R}^{(4)}_{\mu\nu} - \frac{1}{2}R^{(4)}\, g_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi G\, T_{\mu\nu} \tag{2.1}$$

where $\mathcal{R}^{(4)} \in \Gamma(T^0_2\mathcal{M})$ and $R^{(4)} \in \Gamma(T^0_0\mathcal{M})$ denote the Ricci tensor and the four–dimensional curvature scalar respectively, and $G_{\mu\nu}$ the Einstein tensor. They depend on g and the associated unique covariant derivative ∇. We also introduce a cosmological constant $\Lambda \in \mathbb{R}$, and Newton's constant G. These equations need to be postulated but are based on plausible arguments (Carroll

2014): One way to obtain them is to first introduce the Einstein–Hilbert action functional of the gravitational field

$$S_{\mathrm{EH}}[g] = \frac{1}{16\pi G}\int_{\mathcal{M}} \mathrm{d}^4X\sqrt{|g|}\left(R^{(4)} - 2\Lambda\right), \tag{2.2}$$

and to apply the principle of least action. $|g|$ denotes the absolute value of the determinant of the metric tensor. As the matter content, we employ a free real–valued scalar field $\Phi \in \Gamma(T^0_0\mathcal{M})$ (or since Φ is trivial, we simply write $\Phi : \mathcal{M} \to \mathbb{R}$) with a mass $m \in \mathbb{R}^+$ and a quadratic potential. Its action functional is given by (Wald 1984)

$$S_{\mathrm{M}}[g,\Phi] = -\frac{1}{2\lambda}\int_{\mathcal{M}} \mathrm{d}^4X\sqrt{|g|}\left(g^{\mu\nu}\partial_\mu\Phi\partial_\nu\Phi + m^2\Phi^2\right) \tag{2.3}$$

where $\lambda \in \mathbb{R}^+$ is the coupling constant of the scalar field. Note that $1/\lambda$ has dimension of mass squared and we assume it to be of the order of the typical Standard Model particle masses.

The choice of the scalar field serves two purposes: On the one hand, we explore uncharted territory by including quantum mechanical backreaction in the later stages of this work, and therefore refrain from disguising our results by choosing a more complicated matter content. On the other hand, we wish to make contact with cosmological models of the early Universe and follow the concordance theory which introduces a scalar inflaton field as the dominant primordial matter content. To derive Einstein's equations, one can apply the action principle to the total action functional $S = S_{\mathrm{EH}} + S_{\mathrm{M}}$, see for example in the textbooks by Wald (1984) and Carroll (2014). Here, we will however follow the idea by Arnowitt, Deser, and Misner (1959) and perform a foliation of spacetime into (a priori arbitrary) spacelike hypersurfaces before we consider dynamics. Thanks so this splitting (also denoted as ADM formalism due to its inventors), it is possible to define velocities and hence canonical momenta of the basic variables. This is necessary for a Hamiltonian formulation of the problem. In fact, we must follow this Hamiltonian path as we are going to canonically quantize the system later on. We emphasize that this slicing does not break diffeomorphism invariance as the split remains arbitrary. For detailed introductions to the ADM formalism, we refer to the original reference and the books by Wald (1984) and Thiemann (2008), and on which the following section is based.

2.1.1. The ADM Formalism

The ADM split of a four–dimensional spacetime manifold $\mathcal{M}$ requires the latter to have the topology $\mathcal{M} \simeq \mathbb{R}\times\sigma$ where σ is a fixed three–dimensional (spatial) manifold of arbitrary topology. If $\mathcal{M}$ is globally hyperbolic, this is already granted due to a theorem by Geroch (1970). In this work, we assume global hyperbolicity and define the spatial (Cauchy) hypersurfaces $\sigma \simeq \mathbb{T}^3$ to have the topology of flat, compact three–tori. The flatness is supposed to mimic the properties of the concordance cosmological model and the compactness will prevent divergences to appear for the quantum field theory that we consider in the following chapters. Since the radii of the torus can be chosen arbitrarily, it is possible to fix them as the size of the observable Universe such that the model mimics the flatness of the concordance cosmological model while the compactness will prevent divergences to appear for the QFT that we consider in the following chapters.

In the context of the ADM split which we review here following Thiemann (2008), it is useful

to introduce a diffeomorphism $X : \mathbb{R} \times \sigma \to \mathcal{M}$ which maps points $(t, x) \in \mathbb{R} \times \sigma$ to points $X \in \mathcal{M}$. The spatial hypersurfaces σ can be labeled by a global time parameter $t \in \mathbb{R}$ and we will consequently denote them by Σ_t. The "time" vector field $\mathrm{t} \in \Gamma(T^1_0\mathcal{M})$ obeys $\mathrm{t}^\mu \nabla_\mu t = 1$. It is possible to decompose the components of t^μ into its components normal and tangential to Σ_t according to

$$\mathrm{t}^\mu = N n^\mu + \mathcal{N}^\mu \tag{2.4}$$

where $N \in \Gamma(T^0_0\mathcal{M})$ is the lapse function, $\mathcal{N} \in \Gamma(T^1_0\mathcal{M})$ the shift vector and $n \in \Gamma(T^1_0\mathcal{M})$ is the unit normal to Σ_t. The metric tensor $g_{\mu\nu}$ induces a three–dimensional metric $h \in \Gamma(T^0_2(\mathcal{M})$ on the spatial hypersurfaces defined as

$$h_{\mu\nu} := g_{\mu\nu} + n_\mu n_\nu, \tag{2.5}$$

which is spatial in the sense that any contraction of the vectors n^μ, n^ν with $h_{\mu\nu}$ vanishes. In order to introduce a notion of velocity for the spatial metric, it is useful to define the second fundamental form or extrinsic curvature $K \in \Gamma(T^0_2\mathcal{M})$ such that

$$K_{\mu\nu} := h^\rho_\mu h^\sigma_\nu \nabla_\rho n_\sigma = (\mathcal{L}_n h)_{\mu\nu} \tag{2.6}$$

where indices are moved with respect to the original metric $g_{\mu\nu}$, and $K_{\mu\nu}$ is a spatial tensor, too. The second expression introduces the Lie derivative of $h_{\mu\nu}$ with respect to the "temporal" vector n^μ, and hence underlines that $K_{\mu\nu}$ can be interpreted as some kind of velocity of $h_{\mu\nu}$. On the spatial hypersurfaces, it is possible to define a unique, covariant derivative D_μ associated with $h_{\mu\nu}$ with which in turn, we can define a "spatial" curvature tensor $\mathfrak{R}^{(3)} \in \Gamma(T^0_4\mathcal{M})$, Ricci tensor $\mathcal{R}^{(3)} \in \Gamma(T^0_2\mathcal{M})$ and curvature scalar $R^{(3)} \in \Gamma(T^0_0\mathcal{M})$.

To pull tensors back to the spatial hypersurfaces, one employs the three spatial vector fields $X^\mu_a(X) := X^\mu{}_{,a}\,(t, x)|_{X(t,x)=X}$, for example $h_{ab}(t, x) = (X^\mu{}_{,a}\, X^\nu{}_{,b}\, h_{\mu\nu})(X(t, x))$. In total, this permits to express the Einstein–Hilbert and scalar field actions in terms of the variables on the hypersurfaces, the time parameter t as well as lapse N and shift $\mathcal{N}^a$ and which are hence given by

$$\begin{aligned} S_{\mathrm{EH}}[h] &= \frac{1}{16\pi G}\int \mathrm{d}t\,\mathrm{d}^3x\sqrt{|h|}N\left(R^{(3)} + K_{ab}K^{ab} - (K^a_a)^2 - 2\Lambda\right), \\ S_{\mathrm{M}}[h,\Phi] &= \frac{1}{2\lambda}\int \mathrm{d}t\,\mathrm{d}^3x\sqrt{|h|}N\left(\frac{\dot\Phi^2}{N^2} - 2\frac{\mathcal{N}^a}{N^2}\dot\Phi\,\Phi_{,a} - \left(h^{ab} - \frac{\mathcal{N}^a\mathcal{N}^b}{N^2}\right)\Phi_{,a}\Phi_{,b} - m^2\Phi^2\right). \end{aligned} \tag{2.7}$$

2.1.2. Legendre Transform and Dirac Analysis

In this form, the action functional $S = \int \mathrm{d}t\,\mathrm{d}^3x\,\mathcal{L}$, with its Lagrange density $\mathcal{L}$, allow to perform a Legendre transformation and to define conjugate momenta for h_{ab} and Φ as well as a Hamilton and diffeomorphism constraints. In particular, the conjugate momenta of the spatial metric p and the scalar field Π_Φ are defined as (Thiemann 2008)

$$p^{ab} := \frac{\partial\mathcal{L}}{\partial\dot h_{ab}} = \frac{\sqrt{|h|}}{16\pi G}\left(K^{ab} - K\,h^{ab}\right), \qquad \Pi_\Phi := \frac{\partial\mathcal{L}}{\partial\dot\Phi} = \frac{\sqrt{|h|}}{\lambda N}\left(\dot\Phi - \mathcal{N}^a\Phi_{,a}\right) \tag{2.8}$$

with $p \in \Gamma(T^2_{0,1}\mathcal{M})$ and $\Pi_\Phi \in \Gamma(T^0_{0,1}\mathcal{M})$ where the additional index indicates that both fields have density weight $\omega = 1$. On any fixed spatial hypersurface (i.e., for any fixed value of t), the fields $\{h_{ab}, \Phi, p^{ab}, \Pi_\Phi\}$ span the infinite dimensional phase space Γ of the theory. More precisely, Γ is the cotangent bundle $T^*\mathcal{F}$ of the configuration space $\mathcal{F}$ of fields that is spanned by the fields h_{ab} and Φ. Due to the possibly distributional character of the canonical fields, one introduces spatial smearing functions f_1, f_2 on (some chart of) the spatial manifold σ, in order to define the only non–vanishing Poisson brackets on this phase space

$$\{h_{ab}(f_1), p^{cd}(f_2)\} = \delta^c_a \delta^d_b \langle f_1, f_2\rangle, \qquad \{\Phi(f_1), \Pi_\Phi(f_2)\} = \langle f_1, f_2\rangle, \tag{2.9}$$

and where the brackets denote the inner product of the considered smearing function space, e.g., the space of smooth functions with compact support on σ, $C^\infty_0(\sigma)$. Since the velocities of lapse and shift do not occur in the action it is not possible to derive relations that represent them in terms of the fields and their momenta. Rather we obtain the four primary constraints

$$P_N := \frac{\partial \mathcal{L}}{\dot{N}} = 0 =: C_N, \qquad P_a := \frac{\partial \mathcal{L}}{\partial \dot{\mathcal{N}}^a} = 0 =: C_a, \tag{2.10}$$

where we introduced the functions C_N and C_a to emphasize the constraint character of these equations. Obviously, the constraints imply that the canonical fields h_{ab}, N, $\mathcal{N}^a$, p^{ab}, P_N, P_a are not all independent and this requires a special treatment of the dynamical system.

We therefore follow the so–called Dirac analysis given in the textbooks by Henneaux and Teitelboim (1994), Thiemann (2008) and Kiefer (2007), and to which we also refer for more details: In a nutshell, the procedure is similar to the Hamiltonian program for unconstrained field systems in order to define a Hamiltonian density $\mathcal{H}$ and additionally append the primary constraints multiplied with a corresponding set of Lagrange multiplier functions λ_N and λ^a such that

$$\mathcal{H} := \dot{h}_{ab}\, p^{ab} + \dot{\Phi}\Pi_\Phi + \dot{N} P_N + \dot{\mathcal{N}}^a P_a - \mathcal{L} + \lambda_N C_N + \lambda^a C_a. \tag{2.11}$$

In fact, the Hamiltonian is only well defined on a submanifold of the total phase space given by the primary constraints $C_N = 0$ and $C_a = 0$. Since they vanish, they can be added without changing the formalism. The Lagrange multipliers are in principle arbitrary phase space functions but their introduction in the Hamiltonian serves the purpose to properly recover the correct dynamics of the system. Seen as independent variables they ensure that the variational action principle returns the correct equations of motions *including* the primary constraint equations. The total Hamiltonian has the form (Thiemann 2008)

$$\mathbb{H} := \int \mathrm{d}t\, \mathrm{d}^3x \left(N\, H + \mathcal{N}^a H_a + \tilde{\lambda}_N C_N + \tilde{\lambda}^a C_a\right) =: H(N) + \vec{H}(\vec{\mathcal{N}}) + C_N(\tilde{\lambda}_N) + \vec{C}(\vec{\tilde{\lambda}}), \tag{2.12}$$

where we simply merged the arbitrary functions $\dot{N}$, λ_N and $\dot{\mathcal{N}}^a$, λ^a into the new Lagrange multipliers $\tilde{\lambda}_N$ and $\tilde{\lambda}^a$ respectively, and defined H and H_a such that N and $\mathcal{N}^a$ can be extracted as prefactors. Now, the Dirac algorithm proceeds by varying the action with respect to these Lagrange multipliers, and as anticipated, this simply yields the four primary constraints $C_N = 0$ and $C_a = 0$ as can also be read off the Hamiltonian in equation (2.12). To obtain a consistent dynamics, the Dirac algorithm must demand that these constraints are preserved under the evo-

lution of the Hamiltonian. These requirements correspond to evaluating Hamilton's equations for the primary constraints and to require them to vanish for any smearing functions f, $\vec{f}$, namely (Thiemann 2008)

$$\dot{C}(f) := \{\mathbb{H}, C(f)\} = H(f) = 0, \qquad \dot{\vec{C}}(\vec{f}) := \{\mathbb{H}, \vec{C}(\vec{f})\} = \vec{H}(\vec{f}) = 0. \tag{2.13}$$

These secondary constraints imply that the total Hamiltonian is forced to vanish. Checking whether these secondary constraints are preserved under the evolution of the Hamiltonian yields the Dirac or hypersurface deformation algebra evaluated with respect to suitable smearing fields $f_1, f_2, \vec{f}_1, \vec{f}_2$ such that (Thiemann 2008)

$$\{\vec{H}(\vec{f}_1), \vec{H}(\vec{f}_2)\} = -16\pi G\, \vec{H}(\mathcal{L}_{\vec{f}_1}(\vec{f}_2)), \tag{2.14}$$

$$\{\vec{H}(\vec{f}_1), H(f_2)\} = -16\pi G H(\mathcal{L}_{\vec{f}_1} f_2), \tag{2.15}$$

$$\{H(f_1), H(f_2)\} = -16\pi G \vec{H}(\vec{M}(f_1, f_2, h)). \tag{2.16}$$

We see that these equations do not generate new secondary constraints and vanish if the first set of secondary constraints are zero, i.e., the constraints are of first class. We will not discuss these results in more detail as the primary purpose of this section was to present Dirac's algorithm. In chapter 9, we will make explicit use of this algorithm but applied to a cosmological model with appropriate perturbations. This brings us to the topic of our next section.

2.2. The Concordance Lambda–CDM Model

The current concordance model of cosmology (Aghanim et al. 2020a,b; Cervantes–Cota and Smoot 2011; Deruelle and Uzan 2018; Dodelson and Schmidt 2021) is a compilation of physical approaches based on general relativity and the Standard Model of particle physics that intend to interpret and explain cosmological data. Many of its theoretical results are in astonishing agreement with past and present cosmological observations such as the light element abundances that are (to a large extent) in accord with Big Bang Nucleosynthesis (Coc and Vangioni 2017), and the CMB temperature map and power spectra obtained by a multitude of cosmic microwave observations (Aghanim et al. 2020a; Bennett et al. 2013; Leitch et al. 2005; Smoot et al. 1992).

It draws the picture of an ever increasing, statistically and spatially homogeneous and isotropic Universe starting from a dense and hot Big Bang, culminating into the present Universe which is composed of a constant "dark" energy component associated with a cosmological constant Λ ($\sim$ 69% of the total energy budget), cold "dark" matter (CDM, $\sim$ 25%) and baryonic matter ($\sim$ 6%). Despite its achievements, the increasing amount of high–precision measuring data from early Universe surveys such as Planck (Aghanim et al. 2020a), and late time scrutinies such as the Hubble space telescope (Riess et al. 2016) strenghten the doubts regarding our cosmological world view, see for example (Reid, Pesce, and Riess 2019). It is the goal of this section to review the basic ideas of the concordance model with a focus on those aspects relevant for this thesis, as well as to point to its cavities.

2.2.1. Homogeneity and Isotropy

Cosmological data indicates that the Universe has been spatially homogeneous and isotropic up to small perturbations during its earlier phases and when integrated over very large scales (roughly 100 Mpc) today (Dodelson and Schmidt 2021). This is the content of the cosmological principle). One of the most impressive set of results that underlines this hypothesis for the early Universe comes from a multitude of cosmic microwave missions, in particular from the Planck collaboration which offers the most recent and precise temperature map of the observable Universe (Akrami et al. 2020), see Fig. 2.1. The observed photons exhibit an almost perfect black body spectrum with an average temperature of $T = 2.726 \pm 0.001$ K (Fixsen 2009), hence denoted as cosmic microwave background (CMB) radiation. It displays fractional temperature fluctuations of only 10^{-5} which makes the assumption of a purely homogeneous and isotropic Universe plausible. The gravitational field that corresponds to a purely homogeneous and isotropic Universe is the

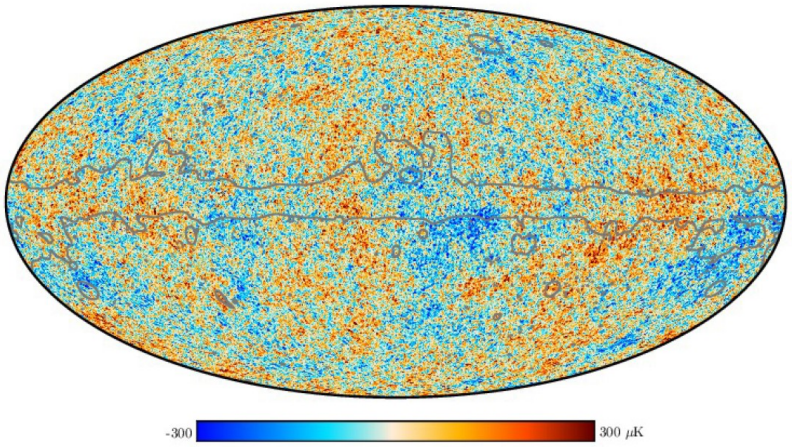

Figure 2.1.: The Planck 2018 CMB temperature map taken from (Aghanim et al. 2020a). Red points indicate slightly hotter and blue points slightly colder spots compared to the mean temperature. The region delineated by a grey line has been masked and inpainted due to residuals from foreground emission.

Friedmann–Lemaître–Robertson–Walker (FLRW) metric given by the line element (Mukhanov 2005)

$$\mathrm{d}s^2 = -N_0\,\mathrm{d}t^2 + a(t)^2\left[\frac{\mathrm{d}r^2}{1-kr^2} + r^2\mathrm{d}\Omega^2\right] =: -N_0\,\mathrm{d}t^2 + h^0_{ab}(t,x)\,\mathrm{d}x^a\mathrm{d}x^b, \tag{2.17}$$

where $\mathrm{d}\Omega$ is the solid angle volume form, r a corresponding radial coordinate, t is cosmic time, and $k \in \{-1, 0, 1\}$ is the curvature parameter defining a hyperbolic, Euclidean or elliptic topology of the spatial hypersurfaces respectively. $a \in \mathbb{R}^+$ is the scale factor which parametrizes the purely homogeneous and isotropic metric. h^0_{ab} denotes the spatial metric induced by the total metric g, where we additonally inserted the superscript "0" to emphasize that we deal with the purely homogeneous and isotropic FLRW metric (without any perturbations). It is often convenient to introduce the time–independent spatial metric $\tilde{h}^0$ on the hypersurfaces according to $h^0(t,x) =: a^2(t)\,\tilde{h}^0(x)$. Following our conventions from the previous section, we set the arbitrary lapse function equal to one, $N_0 \equiv 1$, such that the only remaining dynamical degree of freedom

is the scale factor a. It is often useful to use the conformal time parameter τ defined by $\mathrm{d}\tau := \frac{\mathrm{d}t}{a(t)}$ such that the metric is conformally equivalent to the Minkowski metric up to a global factor $a(\tau)$. Many observations point to a flat Universe with $k = 0$ such as the Planck results combined with data from acoustic baryonic oscillations (Akrami et al. 2020), and we will henceforth adopt this choice. However, we also point to an analysis of the very same CMB data combined with luminosity distance data that excludes this scenario, namely (Di Valentino, Melchiorri, and Silk 2020).

So far, cosmological data supports the idea that the observable Universe is and has been expanding for a very long period of time, i.e., the scale factor has been increasing. As a consequence the physical wavelength of relativistic particles is stretched out and leads to a redshift z defined as (Dodelson and Schmidt 2021)

$$1 + z := \frac{\lambda}{\lambda_{\mathrm{in}}} = \frac{a_0}{a_{\mathrm{in}}}, \tag{2.18}$$

where λ_{in} and a_{in} denote the wavelength and the scale factor at the time when the light is emitted, and $a_0 \equiv 1$ is the scale factor today. Accordingly, light from remote objects is redshifted when it arrives on Earth and provides a mean to estimate their distance and age if the spectrum is known. According to Einstein's equations (2.1), the evolution of the scale factor depends on the matter content of the Universe. A convenient choice for an isotropic and homogeneous Universe is a perfect fluid as it is isotropic in its rest frame. The stress–energy tensor of a perfect fluid with four–velocity u^μ, energy density ρ, and pressure P is given by (Mukhanov 2005)

$$T_{\mu\nu} = (P + \rho)\, u_\mu u_\nu + P g_{\mu\nu}. \tag{2.19}$$

Inserting the FLRW metric (2.17) into both sides of Einstein's equations yields the Friedmann and the Raychaudhuri equations which determine the evolution of the Hubble parameter $H := \frac{\dot{a}}{a}$ and the acceleration of the scale factor respectively (Mukhanov 2005)

$$H^2 = \frac{8\pi G}{3}\rho - \frac{k}{a^2} + \frac{\Lambda}{3}, \qquad \frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho + 3P) + \frac{\Lambda}{3} \tag{2.20}$$

where we included a cosmological constant $\Lambda > 0$. Besides, the conservation of energy, $\nabla_\mu T^{\mu\nu} = 0$, yields the continuity equation for the perfect fluid (Mukhanov 2005)

$$\dot{\rho} + 3H(\rho + P) = 0. \tag{2.21}$$

From now on, we denote quantities that are measured today by a subscript "0" and see how they relate to the quantities at earlier times according to these three equations. By default, one defines and measures the present "critical" energy density using Friedmann's equation (2.20) assuming a flat Universe ($k = 0$) (Dodelson and Schmidt 2021)

$$\rho_{\mathrm{cr}} \equiv \frac{3H_0^2}{8\pi G} = 1.88\, h^2 \times 10^{-29}\,\mathrm{g\,cm^{-3}} \tag{2.22}$$

where the parameter h has been introduced for convenience since H_0 is commonly defined as $H_0 := 100\, h\,\mathrm{km\,s^{-1}Mpc^{-1}}$. Recent analyses yield $h \approx 0.7$ together with a statistically significant disagreement between late and early Universe measurements denoted as the H_0–tension. For example, a combination of data from red giant stars and of Omega Centauri from the Hubble Space Telescope yield $h = 0.72 \pm 0.2$ (Soltis, Casertano, and Riess 2020) while the 2018 Planck

mission attains $h = 0.68 \pm .0$ (Aghanim et al. 2020b). If we allow for a non–vanishing curvature in the Friedmann equation ($k \neq 0$), definition (2.22) implies that a curved Universe has a density ρ_0 today that is *different* from the critical energy density.

2.2.2. Cosmic Inventory

The total energy density $\rho(t)$ at any time is commonly split into different parts according to the constituents that formed the Universe at time t. In the simplest case of a barotropic fluid (i.e., a fluid whose density is a function of pressure only), the behavior of $\rho(t)$ follows from a constant equation of state $P = w\rho$ with $w \in \mathbb{R}$ and the resulting continuity equation (Baumann 2012)

$$\rho = \rho_{\mathrm{in}} \left(\frac{a}{a_{\mathrm{in}}} \right)^{-3(1+w)} \tag{2.23}$$

where ρ_{in} and a_{in} denote the energy density and scale factor at some initial time t_{in}. A gas of non–relativistic matter particles has vanishing pressure ($w = 0$) such that its energy density scales like $\rho_{\mathrm{m}} \sim a^{-3}$, i.e., for an increasing scale factor matter is diluted according to the volume expansion. Radiation has an equation of state $P_{\mathrm{r}} = \frac{1}{3}\rho_{\mathrm{r}}$ such that $\rho_{\mathrm{r}} \sim a^{-4}$ which accounts for the additional energy redshift. The accelerated expansion of the Universe today is attributed to a cosmological constant Λ with $w = -1$, and hence $\rho_\Lambda \sim a^0$. Since it is unclear if this acceleration is soleley driven by a cosmological constant or whether there is an(other) microphyiscal origin, one associates Λ with a "dark energy" component.

We define the dimensionless density parameters $\Omega_{s,0} := \frac{\rho_{s,0}}{\rho_{\mathrm{cr}}}$ for any of the matter species s by dividing by the critical energy density ρ_{cr}, and assume that the respective constituents are non–interacting. Dividing the Friedmann equation by H_0^2 yields (Dodelson and Schmidt 2021)

$$\frac{H^2}{H_0^2} = \Omega_{\mathrm{r},0} \left(\frac{a_0}{a} \right)^4 + \Omega_{\mathrm{m},0} \left(\frac{a_0}{a} \right)^3 + \Omega_{k,0} \left(\frac{a_0}{a} \right)^2 + \Omega_{\Lambda,0}. \tag{2.24}$$

The ΛCDM model includes photons and relativistic neutrinos as radiation as well as baryonic matter, cold dark matter and non–relativistic neutrinos in the matter sector, and we defined density parameters for the curvature $\Omega_{k,0}$ and for the cosmological constant $\Omega_{\Lambda,0}$. The notion of cold dark matter (CDM) was introduced to name a yet unknown (hence "dark") non–relativistic (hence "cold") and gravitationally interacting matter component present in the Universe (Blumenthal et al. 1984). The Planck collaboration determined values for these parameters (within the 68% confidence limit) using the CMB data as well as measurements from recent galaxy surveys such as SDSS, 2dFGRS and many more given by (Aghanim et al. 2020b)

$$\Omega_{\Lambda,0} = 0.689 \pm 0.006, \quad \Omega_{\mathrm{m},0} = 0.311 \pm 0.006, \quad \Omega_{k,0} = 0.001 \pm 0.002, \quad \Omega_{\mathrm{r},0} \leq 10^{-4}. \tag{2.25}$$

Consequently, the standard baryonic matter represents only about 6% of the total energy density contributions while the remaining matter part is attributed to a CDM component. According to Friedmann's equation (2.24), the relative abundances of the components have changed during the evolution of the Universe. Using the formula for the redshift together with Friedmann's law (2.24) and the parameters (2.25), it is straightforward to deduce the redshift at which dark matter starts

to dominate over cold matter, and the redshift when matter begins to dominate over radiation. In particular, we have that (Aghanim et al. 2020b)

$$z_{\Lambda-\mathrm{m}} = \left(\frac{\Omega_\Lambda}{\Omega_\mathrm{m}}\right)^{\frac{1}{3}} - 1 \approx 0.30, \qquad z_{\mathrm{m}-\mathrm{r}} = \left(\frac{\Omega_\mathrm{m}}{\Omega_\mathrm{r}}\right) - 1 \approx 3380. \tag{2.26}$$

There is yet another possibility to identify epochs and events of cosmic history which is particularly useful as is extends to phases prior to radiation domination and the release of the CMB photons. Wien's displacement law stipulates the ratio of the peak of the black body frequency and the corresponding temperature to be a constant such that the temperature T at some time t is given by $T(t) = T_0 \cdot (\nu(t)/\nu_0) = T_0/a(t) = 2.726\,\mathrm{K} \cdot (1 + z(t))$.

2.2.3. Cosmic Evolution

The Friedmann equation reveals that the first dominant energy component among the ones given in equation (2.25) in an expanding Universe with non–interacting constituents must have been relativistic radiation, followed by a period with non–relativistic matter preeminence. In our Universe, the curvature density parameter is to small to yield a nominal effect such that the subsequent phase (today) is dark energy–dominated. This recent epoch sees the formation of a rich structure of galaxies and clusters due to the gravitational force that drives the accumulation of matter in an elsewhere rather empty and expanding Universe. The following chronology is based on (Mukhanov 2005; Wikipedia 2020).

At redshift $z_{\Lambda-\mathrm{m}} \approx 0.3$ ($T \approx 3.5$ K), going backwards in time, the matter components took over and prepared the present structure formation. The first stars were born at around $z \approx 16$ ($T \approx 46$ K) which gave rise to the phase of reionization due to the intense radiation they emitted. The first galaxies formed at $z = 11.1$ ($T = 33$ K) (Oesch et al. 2016). Prior to reionization, there were no light–emitting structures yet which led to the notion of the "Dark Ages". At these times, the Universe had cooled down enough to allow photons to travel long distances and in fact, the Universe was pervaded by a radiative background which would later form the CMB. The photons decoupled at around $z \approx 1090$ ($T \approx 3000$ K) from the hot and dense plasma of baryonic and dark matter which itself began to recombine to neutral atoms. This epoch sees the formation of the cosmic web driven by the presence of dark matter that acts gravitationally and which reinforces the already existing density fluctuations in the hot plasma.

The matter–dominated era passes into a phase of radiation supremacy at around $z \approx 3600$ ($T \approx 10^4$K). The high temperatures allowed for nuclear fusion to occur which ushers in the era of Big Bang Nucleosynthesis, producing light elements like hydrogen ($\sim 75\%$), helium ($\sim 25\%$) and negligible parts of lithium at around $T = 10^7\mathrm{K} - 10^9\mathrm{K}$. The predicted relative abundances of these elements can be tested against observational data from galaxies and provide yet another impressive confirmation of the standard hot Big Bang model, despite the yet unsolved discrepancy of the lithium abundance between measurements and predictions by a factor of 3 (Coc and Vangioni 2017). Prior to this phase, the Universe was presumably and dominantly filled with leptons and neutrinos ($T = 10^7\mathrm{K} - 10^9\mathrm{K}$). The decoupling of the latter species produced a cosmic neutrino background that is observable today (at least indirectly in the CMB patterns) (Follin et al. 2015). Aforetime, hadrons started to be produced as the Universe cooled down to temperatures of 10^{10}K

– 10^{12}K, and made up the dominant energy contribution before even lower temperatures prevented their production. The hadron epoch was preceded by the quark epoch during which the Universe's temperature of 10^{12}K – 10^{15}K were too high to allow the formation of hadrons from the dense quark–gluon plasma that pervaded the Universe. The quark epoch had followed the phase of electroweak symmetry breaking that occured at $T \approx 10^{15}$K and presented the end of the thermalization phase during which the first particles interacted such that a thermal equilibrium was achieved. This era is denoted as the electroweak epoch and roughly encounters temperatures between 10^{22}K and 10^{29}K.

Physics prior to this epoch is still very speculative. The standard Hot Big Bang model assumes that the mentioned particles have been produced by a decaying real scalar field that dominated the Universe during its very first moments. This is the inflaton field, and the corresponding "inflationary" phase is claimed to provide answers to some of the open questions of the standard hot Big Bang model.

2.2.4. Problems of the Lambda–CDM Model

The ΛCDM model as presented above implies a number of odd results. One of these problems concerns the apparent isotropy of the CMB radiation which leads us to assume that CMB photons from any direction arriving today on Earth must have thermalized at earlier times, i.e., must have been in causal contact. To verify this assumption, we evaluate the angle between two points (photons) in the CMB radiation map that had the possibility to causally interact from the presumed beginning of the Universe until photon decoupling (last scattering) at $a_{\mathrm{ls}} \approx (1 + z_{\mathrm{ls}})^{-1} \approx 10^{-3}$. Since photons follow null rays their maximal radial comoving distance Δx they can cover equals the conformal time $\Delta\tau$ that has passed. Between an initial time $t = t_{\mathrm{in}}$ and the time of last scattering t_{ls}, a photon could hence have covered the comoving distance (Baumann 2012)

$$\Delta x =: \chi_{\mathrm{ph}}(t_{\mathrm{ls}}) = \int_{t_{\mathrm{in}}}^{t_{\mathrm{ls}}} \frac{\mathrm{d}t}{a(t)} = \int_{a_{\mathrm{in}}}^{a_{\mathrm{ls}}} \frac{\mathrm{d}a}{H(a)a^2} \tag{2.27}$$

which is precisely the particle horizon χ_{ph} of a photon at t_{ls}, i.e., the maximal distance from where the photons can receive light signals given the Universe "begins" at $t = t_{\mathrm{in}}$. This corresponds to a physical distance $l = a_{\mathrm{ls}} \cdot \chi_{\mathrm{ph}}(t_{\mathrm{ls}})$ at the time of last scattering. Two photons seperated by that distance at t_{ls} might have travelled towards us and the comoving distance they covered if they arrive today is (Baumann 2012)

$$\chi_{\mathrm{eh}}(t_0) := \int_{t_{\mathrm{ls}}}^{t_0} \frac{\mathrm{d}t}{a(t)} = \int_{a_{\mathrm{ls}}}^{a_0} \frac{\mathrm{d}a}{H(a)a^2}, \tag{2.28}$$

which is the photon's event horizon $\chi_{\mathrm{eh}}(t_0)$, i.e., the maximal distance they could have traveled until today. The comoving particle and the event horizons can be computed explicitely using those two formulae and equation (2.24) assuming that we evaluate it before dark energy dominates. Using the parameters (2.25) shows that $\chi_{\mathrm{ph}} \ll \chi_{\mathrm{eh}}$ such that the small angle–approximation is valid in order to infer the angle through which we observe a formerly causally connected patch in

the CMB map, namely (Mukhanov 2005)

$$\Theta = \frac{l}{d_\mathrm{A}} := \frac{\chi_\mathrm{ph}(t_\mathrm{ls})}{\chi_\mathrm{eh}(t_0)} \approx 0.019\,\mathrm{rad}, \tag{2.29}$$

where we implicitely stated the standard formula for the angular diameter distance d_A. This corresponds to an angle of 1.1°, and consequently a sky consisting of $\frac{4\pi}{0.019^2} \approx 3 \times 10^4$ causally disconnected patches which seems implausible given the high degree of isotropy in the CMB map. A possible solution to this problem becomes apparent by rewriting the integral in equation (2.27) using the logarithm of the scale factor as,

$$\chi_\mathrm{ph}(t_\mathrm{ls}) = \int_{\ln a_\mathrm{in}}^{\ln a_\mathrm{ls}} (aH)^{-1} \mathrm{d} \ln a. \tag{2.30}$$

Any process between the initial time t_in and last scattering that leads to a decreasing Hubble radius $(aH)^{-1}$ (the comoving distance which particles can travel during the time $\frac{\mathrm{d}t}{\mathrm{d}\ln a}$) would *increase* the particle horizon and hence ease the causality problem which is also known as the horizon problem. This requirement can be achieved by a phase of accelerated expansion $\ddot{a} > 0$ during which the scale factor grows by a factor e^N with $N := \ln(a_\mathrm{e}) - \ln(a_\mathrm{in})$ being the number of e–folds (Baumann 2012).

Another peculiarity of the ΛCDM model is the so–called flatness problem which results from the present density parameter $\rho(t_0)$ being very close to the critical density ρ_cr. This means that the reduced density $\Omega(t_0) := \frac{\rho(t_0)}{\rho_\mathrm{cr}}$ is very close to unity. In fact, this also implies that the density parameter $\Omega(t)$ must have been very close to unity throughout its entire history which seems a very ad hoc assumption given its diverse history. Since the actual density $\Omega(t)$ of the Universe at some previous moment in time $t < t_0$ differs from the critical density $\Omega_\mathrm{cr} = 1$ by the curvature term $\Omega(t) - 1 =: \Omega_k(t) = k \cdot (aH)^{-2}$ with k being constant, the critical curvature density at any time t is given by (Mukhanov 2005)

$$\Omega_k(t) = (\Omega(t_0) - 1)\frac{(a_0 H_0)^2}{(a(t)H(t))^2} = (\Omega(t_0) - 1)\frac{\dot{a}_0^2}{\dot{a}(t)^2}. \tag{2.31}$$

We evaluate this expression for the early radiation dominated Universe for which we have $\dot{a}_0 \cdot \dot{a}(t)^{-1} \sim a(t) \cdot a_0^{-1}$ according to Friedmann's equation. We consider the era of electroweak symmetry breaking as the first phase of which cosmologists are relatively certain and assume that the scale factor was smaller by a factor 2.726×10^{-29} as it is today such that $\Omega_k(t_\mathrm{ew}) \leq 7 \times 10^{-62}$. This small value is difficult to reconcile with a cosmologist's idea of a "natural" cosmological parameter. From equation (2.31) it follows that a very large Hubble radius $(aH)^{-1}(t_\mathrm{in})$ at some earlier time t_in provides a mean to allow for a larger value of $\Omega_k(t_\mathrm{ew})$. If succeeded by a phase with decreasing Hubble radius, this procedure provides a mechanism to have a very small density parameter at t_ew without choosing the value by hand.

Both the horizon and the flatness problem prefigure a phase of accelerated expansion at earliest times during which the Hubble radius should decrease substantially. A similar mechanism has also been proposed regarding the so–called monopole problem which occurs when including a very early epoch of Grand Unification of forces (i.e., an early period at which the temperature

was so high that the electroweak and the strong force were unified as the electronuclear force) . Such a phase would produce a high abundance of massive monopoles during symmetry breaking which in turn would imply a monopole density of at least 10^{13} times the critical density today (Mukhanov 2005). This is in obvious disagreement with cosmological data. As anticipated before, a long enough lasting period of accelerated expansion would dilute the monopole's number density such that it drops to only one monopole per present horizon scale. The current concordance model of cosmology invokes a real–valued scalar field Φ with a potential energy $V(\Phi)$ and which is able to drive a phase of such accelerated expansion.

2.2.5. Inflation

The simplest inflationary model enriches the cosmic inventory by a real–valued scalar field $\Phi \in \Gamma(T^0_0\mathcal{M})$ with a quadratic potential and an action S_M given in equation (2.3). Assuming that the field has been spatially homogeneous and isotropic on the constant cosmic time hypersurfaces, the action reduces to (Baumann 2012)

$$S_\mathrm{M}[\phi] = \frac{1}{2\lambda}\int \mathrm{d}t\, a^3 \left(\dot{\phi}(t)^2 - m^2\,\phi(t)^2\right) \tag{2.32}$$

where we distinguish the time–dependent homogeneous and isotropic field $\phi : \mathbb{R} \to \mathbb{R}$ from the generic space and time–dependent field Φ. The principle of least action yields the stress–energy tensor $T_{\mu\nu}$ by varying the action S_M with respect to the metric tensor $g_{\mu\nu}$. Comparing the resulting tensor to the standard stress–energy tensor of a perfect fluid in the homogeneous and isotropic case (cf. equation (2.19)) yields an equation of state (Baumann 2012)

$$w = \frac{P}{\rho} = \frac{\dot{\phi}(t)^2 - m^2\,\phi(t)^2}{\dot{\phi}(t)^2 + m^2\,\phi(t)^2}. \tag{2.33}$$

The Raychaudhuri equation (2.20) for an inflaton Universe indicates that a phase of accelerated expansion with $\ddot{a} > 0$ requires that $w < -\frac{1}{3}$. In this case, we infer from equation (2.33) that the potential energy of the field must dominate over the kinetic energy. In cosmology, it is common to use the so–called slow–roll approximation to guarantee a phase of accelerated expansion by assuming that $\dot{\phi}^2 \ll m^2\,\phi^2$ such that $w \approx -1$. This corresponds to a dynamical phase with a large potential energy and a vanishing kinetic energy, hence the name "slow–roll". In such a case, the continuity equation for a perfect fluid reduces to $\dot{\rho} \approx 0$ and Friedmann's equation consequently yields a constant Hubble parameter H such that

$$a(t) = a_\mathrm{in}\, e^{H(t-t_\mathrm{in})}. \tag{2.34}$$

Consequently, inflation generates a de Sitter–like expanding Universe, i.e., a Universe with a constant exponential expansion. To obtain a sufficient amount of inflationary e–folds, this expansion must persist long enough. This requirement together with the first slow–roll condition from above is usually expressed using the so–called slow roll parameters ϵ and η (Baumann 2012)

$$\epsilon := \frac{4\pi G\dot{\phi}^2}{H^2} \ll 1, \quad \eta := \frac{\dot{\epsilon}}{H\epsilon} \ll 1 \tag{2.35}$$

which should remain small and constant during inflation. Knowing that H remains unchanged during inflation and that a grows exponentially, the flatness problem (2.31) gives an estimate on how many e–folds are necessary to outweigh the very small factor $(a_0H_0)^2(a(t)H(t))^{-2} \approx 7{\times}10^{-58}$ which led to $\Omega_k(t) \leq 7 \times 10^{-62}$. In particular, this requires the number of e–folds to be $N \geq \ln\left(10^{29}/2.726\right) \approx 66$. An inflationary model which is capable of generating this number of e–folds would as well solve the horizon and the monopole problem (Mukhanov 2005). Providing such a phase of accelerated expansion was the motivating idea behind the inflationary model, and its simplicity gave the theory soon its present standing in the cosmological concordance theory.

Another important feature of the inflationary model is that it provides a natural mechanism to account for the observed large scale structure of the present Universe and the tiny perturbations in the CMB temperature map. The idea is to introduce very small perturbations of the inflaton and the metric field that are presumably caused by inhomogeneous quantum fields at earliest times. The homogeneous part of the inflaton would stretch these perturbations to horizon scales while a suitable mechanism (e.g., decoherence (Schlosshauer 2007)) renders the perturbations classical. This would lead to the rich cosmic structure of our present Universe. Since these perturbations depend on both space and time coordinates they introduce a gauge arbitrariness due to the underlying diffeomorphism invariance of general relativity.

2.2.6. Cosmological Perturbations

The basic idea underlying standard cosmological perturbation theory is on the one hand to assume that it is physically meaningful to foliate space time into certain spatial hypersurfaces Σ_t, $t \in \mathbb{R}$, on which it is admissible to consider the cosmological fields as maximally symmetric, i.e., as homogeneous and isotropic. This corresponds to the assumptions of the cosmological principle, namely that the geometry of the Universe admits a purely spatially homogeneous and isotropic solution associated with a spatially homogeneous and isotropic matter content. On the other hand, cosmological perturbation theory allows for small inhomogeneities. This motivates the following split for any cosmological field $\vartheta^a(t,x)$, $a = 1, 2, \ldots$, such as the components of the metric tensor $g_{\mu\nu}$ or the scalar field Φ (Abramo, Brandenberger, and Mukhanov 1997)

$$\vartheta^a(t,x) =: \vartheta^a_0(t) + \delta\vartheta^a(t,x). \tag{2.36}$$

The first contribution $\vartheta^a_0(t)$ is obtained by a maximal symmetry reduction of the total fields $\vartheta^a(t,x)$ (for example, the FLRW metric), and provides a solution for an actual spatially homogeneous and isotropic Universe. It is often assumed that the functions ϑ^a_0 result from a spatial averaging of the fields $\vartheta^a(t,x)$. By definition, they depend only on time. The scale factor $a(t)$ would be one example. The second part represents a small linear perturbation of the homogeneous and isotropic solution ϑ^a_0. They are required to be small in the sense that $|\delta\vartheta^a| \ll |\vartheta^a_0|$ for any scalar component ϑ^a.

To be more precise, we introduce a set of perturbation fields of the metric and the scalar field following the notation by Castelló Gomar, Martín-Benito, and Mena Marugán (2015) as we are going to make use of their results when it comes to gauge–invariant perturbation theory in chapter 9. Their notation differs from the standard one, used for instance in the textbook by Peter and

Uzan (2009) and the article by Ma and Bertschinger (1994) but turns out to have advantages for the pursued Dirac analysis (the difference basically consists in adding factors of $a(t)$ and covariant derivatives at various places). It is useful to decompose the perturbations into its scalar, vector and tensor components with respect to three–dimensional rotations since at linear perturbative order the perturbations will decouple. The perturbed FLRW metric element then has the form

$$\begin{aligned} \mathrm{d}s^2 =& -(N_0 + a^3\eta(t,x))\,\mathrm{d}t^2 + 2a^2(D_a k(t,x) + \epsilon_a^{bc} D_b k_c(t,x))\,\mathrm{d}x^a\mathrm{d}t \\ &+ a^2\left[(1+\alpha(t,x))\tilde{h}^0_{ab} + 6\left(D_aD_b - \frac{\tilde{h}^0_{ab}}{3}\Delta\right)\beta(t,x) + 2\sqrt{6}t_{ab}(t,x) + 4\sqrt{3}D_{(a}v_{b)}(t,x)\right]\mathrm{d}x^a\mathrm{d}x^b \end{aligned} \tag{2.37}$$

where $\Delta := D_aD^a$ is the Laplace–Beltrami operator on the spatial hypersurface. It includes a lapse perturbation η, the shift perturbation k and the spatial perturbation fields α and β in the scalar sector. The vector perturbations are incorporated in the shift vector by the function k_a and in the spatial metric by v_a. The tensorial perturbations are denoted by t_{ab}. The matter scalar field splits up into a homogeneous and an inhomogeneous part according to $\Phi(t,x) =: \phi(t) + \varphi(t,x)$.

The choice of field degrees of freedom in this representation is obviously redundant as the number of variable fields is higher than the number of physical fields (recall that the metric tensor has a totality of only two physical degrees of freedom), ergo there is a gauge choice to be made. One possibility is to set several of the fields equal to zero which is particularly convenient when a choice of spatial hypersurfaces is physically prescribed and fixed. If the possibility of coordinate (or rather gauge) transformations should be kept open and in order to prevent fictitious unphysical perturbations when changing the gauge, it is advisable to introduce a set of gauge–invariant perturbation variables. Regarding the tensor sector, t_{ab} is already gauge invariant. In the scalar sector, the real–valued Mukhanov–Sasaki field ϑ represents the standard choice for a gauge invariant field (Kodama and Sasaki 1984; Mukhanov 1988, 2005)

$$\vartheta := a\left(\varphi - \frac{a\dot{\phi}}{H}(\alpha - \Delta\beta)\right). \tag{2.38}$$

For the time being, we omit the discussion of the vector perturbations as they are not relevant for our later results. The remaining scalar functions η and k associated with lapse and shift perturbations are Lagrange multipliers and can hence be chosen arbitrarily. Knowing the evolution of the remaining dynamical fields will allow to relate the primordial perturbations to the matter and CMB fluctuations today.

2.2.7. Evolution of Perturbations

The dynamics of the physical perturbation fields $\delta\theta^a$ result from inserting the ansatz $\theta^a_0 + \delta\theta^a$ for the cosmological quantities into Einstein's equations. The latter will be written in shorthand notation as

$$\Pi[\theta^a] \equiv \Pi_{\mu\nu}[g,\Phi] := G_{\mu\nu}[g] - 8\pi G T_{\mu\nu}[g,\Phi] = 0 \tag{2.39}$$

where the Einstein and stress–energy tensor are to be understood as functionals of g and Φ. The standard cosmological reasoning goes as follows (Mukhanov, Feldman, and Brandenberger 1992):

1. Expand Einstein's equations in a functional power series in $\delta\theta^a$ about the background θ^a_0

(Abramo, Brandenberger, and Mukhanov 1997)

$$\Pi[\theta_0] + \Pi_{,a}[\theta_0]\delta\theta^a + \frac{1}{2}\Pi_{,ab}[\theta_0]\delta\theta^a\delta\theta^b + \mathcal{O}(\delta\theta^3) = 0 \tag{2.40}$$

where $\mathcal{O}(\delta\theta^3)$ subsumes any contribution of third or higher order in the perturbative fields, and a comma stands for the derivative with respect to the perturbative field.

2. Assume that the homogeneous and isotropic fields θ_0^a solve Einstein's equations such that $\Pi[\theta_0] = 0$ holds true *independently* of the remaining perturbative expressions.

3. Assuming that quadratic and higher perturbative terms are negligible compared to the linear ones, and that the Friedmann equations from the previous step are satisfied, the linearized equations of motion for the cosmological perturbations read

$$\Pi_{,a}[\theta_0]\delta\theta^a = 0. \tag{2.41}$$

   Insert the solutions of the homogeneous Friedmann equations into equation (2.41) and solve for the perturbative degrees of freedom. The result is a set of second order differential equations (2.42) for the perturbations that depend (non–linearly) on the (fixed) "background" Friedmann solutions.

4. Omit any higher order contributions of the perturbed Einstein equations.

Following this procedure, it is straightforward, although lengthy, to derive the concrete form of the perturbative equations of motion (2.41), and we therefore refer to the seminal work by Mukhanov, Feldman, and Brandenberger (1992). For stating the results, we note that the tensor perturbations carry only two independent degrees of freedom corresponding to their two polarizations and we label these fields by $t_\pm$. Besides, it is convenient to use the conformal time parameter τ instead of cosmic time t, and the time–dependent function $\zeta := a\frac{\dot{\phi}}{H}$ where H is the Hubble parameter. This gives the three differential equations for the Mukhanov–Sasaki field ϑ and the two tensor polarizations $t_\pm$ (also known as gravitational waves):

$$\frac{\mathrm{d}^2\vartheta}{\mathrm{d}\tau^2} - \left(\Delta + \frac{1}{\zeta}\frac{\mathrm{d}^2\zeta}{\mathrm{d}\tau^2}\right)\vartheta = 0, \qquad \frac{\mathrm{d}^2 t_\pm}{\mathrm{d}\tau^2} - \left(\Delta + \frac{1}{a}\frac{\mathrm{d}^2 a}{\mathrm{d}\tau^2}\right)t_\pm = 0. \tag{2.42}$$

Both equations resemble the standard Klein–Gordon field equations with a *time–dependent* mass, and they differ precisely in the form of this mass term. Without loss of generality, let us focus on the case of the scalar modes here.

Before we continue with the solutions, let us note that instead of deriving the equations of motions for the (scalar) perturbations by inserting the perturbed fields into Einstein's equations, one can start with the action functional of the gravity–matter system and insert the perturbed fields at this level. The part of the action associated with the perturbative Mukhanov–Sasaki variables is given by the second order matter action (Mukhanov 2005)

$$S_{\mathrm{M}}[\vartheta]|_2 = \frac{1}{2}\int_\sigma \mathrm{d}^3x \left((\vartheta')^2 + \vartheta\left(\Delta + \frac{\zeta''}{\zeta}\right)\vartheta\right) \tag{2.43}$$

where the prime denotes a derivative with respect to conformal time τ. The corresponding Hamil-

tonian obtained by a Legendre transformation with canonically conjugate momentum $\pi_\vartheta := \frac{\partial \mathcal{L}_M|_2}{\partial \vartheta'} = \vartheta'$ of ϑ is given by

$$H_M|_2 = \frac{1}{2}\int_\sigma \mathrm{d}^3x \left(\pi_\vartheta^2 + \vartheta\left(-\Delta + \frac{\zeta''}{\zeta}\right)\vartheta\right) \tag{2.44}$$

where $\mathcal{L}_M|_2$ is the Lagrange density associated with the second order perturbative action $S_M|_2$. The transition to a Hamiltonian description is most useful since the standard cosmological paradigm considers the perturbative fields as quantum fields at earliest times (on a cosmological classical background), and hence the procedure makes it possible to directly perform a canonical quantization. Therefore, one imposes the standard field commutation relations evaluated for two smearing fields $f_1, f_2 \in \mathcal{S}(\sigma)$:

$$[\boldsymbol{\vartheta}(f_1), \boldsymbol{\pi}_\vartheta(f_2)]_{\mathrm{pert}} = i\,\langle f_1, f_2\rangle\, \mathbf{1}_{\mathrm{pert}}, \tag{2.45}$$

and all other commutators are vanishing. The quantum fields $\boldsymbol{\vartheta}$ and $\boldsymbol{\pi}_\vartheta$ belong to the algebra of quantum fields $\mathcal{A}_Q$. The commutator defined on this algebra obviously acts on the only dynamical degrees of freedom – the perturbative fields. The angle brackets denote the inner product of the function space $\mathcal{S}(\sigma)$ and $\mathbf{1}_{\mathrm{pert}}$ denotes the one of the perturbative field operator algebra. We will review the basics of QFT on CST in chapter 4 in more detail.

In order to gain insights into the structure of solutions, it is useful to use standard annihilation and creation operators $\boldsymbol{a}$ and $\boldsymbol{a}^*$ which are linear functions of the canonical field operators. These are usually introduced by expanding the canonical fields with respect to a mode basis, i.e., a set of normalized solutions to the classical field equations (2.42) (Mukhanov 2005). Since the underlying FLRW space time is conformally static, time and space variables can be separated in a suitable ansatz function for the solutions. In the spatially flat case, the solutions of the spatial equation are the standard plane waves labeled by the wave vectors $k_d \in \mathbb{R}^3$ (Fulling 1989). For simplicity, we will omit spatial indices for the coordinates x and the wave vectors k and denote products simply by $k_d x^d =: kx$.

The temporal solutions of the field equations are the corresponding Fourier modes $v_k(\tau)$ which obey a standard oscillator equation with time–dependent frequency $\omega_k^2 = k^2 - \frac{1}{\zeta}\frac{\mathrm{d}^2\zeta}{\mathrm{d}\tau^2}$, see equation (2.47). Since the differential equation is of second order, there are two independent solutions for every k^2 associated with k and $-k$. Hence, the quantum field can be decomposed according to (Baumann 2012)

$$\boldsymbol{\vartheta}(f) = \int_{\mathbb{R}} \frac{\mathrm{d}^3k}{(2\pi)^{3/2}} \left(\boldsymbol{a}_k\, \overline{v}_k(\tau)\check{f}_{-k} + \boldsymbol{a}_k^*\, v_k(\tau)\check{f}_k\right) \tag{2.46}$$

where we introduced the spatial smearing function $f \in \mathcal{S}(\sigma)$ and its Fourier transform $\check{f} \in \mathcal{S}(\sigma)$. Besides, $v_k : \mathbb{R} \to \mathbb{C}$ is a complex–valued function and the bar denotes complex conjugation. The $\boldsymbol{a}_k^*$ denotes the adjoint of $\boldsymbol{a}_k$. Note that this map actually underlies a representation map and we will be more precise in chapter 4 but remain here with the standard proceeding in cosmology. Besides, we used that for a real–valued scalar field $\vartheta(\tau, x)$, the mode functions satsify $v_k(\tau) =$

$\overline{v}_{-k}(\tau)$. Then, the temporal mode functions $v_k(\tau)$ must satisfy (Baumann 2012)

$$\frac{\mathrm{d}^2 v_k}{\mathrm{d}\tau^2} + \left(k^2 - \frac{1}{\zeta}\frac{\mathrm{d}^2\zeta}{\mathrm{d}\tau^2}\right) v_k = 0 \tag{2.47}$$

as well as the (Wronskian) normalization condition (Baumann 2012)

$$(v_k)'\,\overline{v}_k - v_k\,(\overline{v}_k)' = 2i. \tag{2.48}$$

Then, the standard commutation relations for the annihilation and creation operators have the only non–vanishing commutator

$$[\boldsymbol{a}(f_1), \boldsymbol{a}^*(f_2)]_{\mathrm{pert}} = \langle f_1, f_2\rangle\, \mathbf{1}_{\mathrm{pert}} \tag{2.49}$$

where the smearing functions f_1 and f_2 are chosen as above. We emphasize that in this picture, the quantum fields carry the time dependence while the states of the theory are defined to be time–independent. This is the Heisenberg picture, commonly used in cosmological applications. Later on, we will also use the Schrödinger picture in which the states are time–dependent, not the operators.

Having defined the annihilation and creation operators by means of their commutation relations, one can construct an appropriate Hilbert space (for example a Fock space). The vacuum state Ω is defined as the state that is annihilated by any of the annihilation operators, i.e., $\boldsymbol{a}(f)\Omega = 0$, $\forall f \in \mathcal{S}(\sigma)$, and any excited state can be constructed by an appropriate application of creation operators on the vacuum. However, the physical content of the theory and the physical interpretation of the states becomes clear only after fixing the mode functions v_k (Mukhanov and Winitzki 2007). In fact, a different choice of normalized mode functions u_k that is related to the v_k's and v_k^*'s by a simple linear transformation

$$u_k = \alpha_k v_k + \beta_k \overline{v}_k, \quad \alpha_k, \beta_k \in \mathbb{C}\ \forall k \in \mathbb{R}^3,\ |\alpha_k|^2 - |\beta|^2 = 1 \tag{2.50}$$

gives rise to a new set of annihilation and creaction operators given by

$$\boldsymbol{b}_k = \alpha_k \boldsymbol{a}_k - \beta_k \boldsymbol{a}_{-k}^*, \quad \boldsymbol{b}_k^* = \overline{\alpha}_k \boldsymbol{a}_k^* - \overline{\beta}_k \boldsymbol{a}_{-k}. \tag{2.51}$$

The linear coefficients α and β are known as the Bogoliubov coefficients (Bogoliubov 1958). One can easily deduce that the mean density of particles of the v–representation in the vacuum state of the u–representation is given by, $\int \mathrm{d}^3k|\beta_k|^2$ (Mukhanov and Winitzki 2007). This density is only finite if $|\beta_k|^2$ decays faster than k^{-3} for large k. If this is not the case the Bogoliubov transformations are not well–defined and it is not possible to express the one vacuum state by means of excited states in the other representation.

All the choices of mode functions are a priori equivalent, or rather, there is no preferred choice of mode solutions inherently given by the theory. However, in order to make physical predictions or to compare to physically relevant results, it is of course vital to choose a certain representation, i.e, a set of mode functions. As seen above, this choice is tantamount to a choice of vacuum and correspondingly excited states. Unfortunately, in general curved space times, there

is no preferred choice of normalized mode functions, and hence no preferred vacuum state. The notion of a preferred vacuum state is only available in highly symmetric situations. For example in Minkowski space time, the Poincaré symmetries unambiguously fix such a set of mode functions for a quantum field with a certain mass which is hence associated with a physical vacuum state (namely the state that is invariant under Poincaré transformations) and the corresponding excited particles. Note that the vacua for fields with different masses remain unitarily inequivalent even in this highly symmetric scenario. Similarly, in de Sitter space time the Bunch–Davies vacuum is the physically preferred vacuum state for a matter quantum field of a certain mass. In general curved space times, possibly without any symmetries, such a criterion is missing, and hence, the choice of mode functions is ambiguous. There are however certain physically reasonable criteria that allows one to choose a set of mode functions rather than others.

One possibility is to fix an "instantaneous" vacuum state for some particular time $\tau = \tau_0$ (Mukhanov and Winitzki 2007). The idea is to fix the initial conditions for a set of mode functions with respect to which the Hamilton operator $\boldsymbol{H}$ has a minimal expectation value in the corresponding vacuum state. These initial conditions are given by $v_k(\tau_0) = \omega_k(\tau_0)^{-1/2}\exp(i\alpha_k(\tau_0))$ and $v_k'(\tau_0) = i\omega_k(\tau)v_k(\tau_0)$ where $\alpha_k(\tau_0) \in \mathbb{R}$ is a free parameter. Hence, this prescription does not fix the freedom in the initial conditions completely. In the case that $\omega_k^2(\tau_0) < 0$, such an instantaneous vacuum does not exist. Besides, the instantaneous vacuum at any other time $\tau_1 \neq \tau_0$ will be different from the one at τ_0.

Another useful notion of the vacuum is available in space times with a slowly changing gravitational field, more precisely, when the frequencies $\omega_k(\tau)$ are varying slowly. The construction of these so–called adiabatic vacuum state relies on a WKB approximation for the ansatz solutions of the mode functions accordingly given by (Parker 1969)

$$v_k(\tau) = \frac{1}{\sqrt{W_k(\tau)}}\exp\left[i\int_{\tau_0}^{\tau} \mathrm{d}\tau W_k(\tau)\right], \tag{2.52}$$

and which must obey the mode equations of motion (2.47). One expands W_k in powers of the small parameter $(\omega_k T)^{-1}$ where T is a fixed time interval within which ω_k and all its derivatives do not vary substantially. This gives a perturbative scheme for determining the adiabatic mode functions v_k and their initial values $v_k(\tau_0)$ and $v_k'(\tau_0)$. It was shown that the adiabatic states of fourth order in this perturbative scheme can regularize the stress–energy tensor of the free theory and are thus physically reasonable states (Lindig 1999) (we will be more precise on this topic in chapter 4). We point out that similar to the instantaneous vacuum state, the adiabatic vacuum states depend on the precise choice of an initial time τ_0, and are thus still ambiguous. Finally, we mention that Agullo, Nelson, and Ashtekar (2015) have introduced another notion of a preferred instantaneous vacuum state for FLRW cosmologies for which every Fourier mode makes a vanishing contribution to the adiabatically renormalized stress–energy tensor. Here as well, the vacuum choice depends on the moment τ_0 at which the initial conditions are set.

In short, due to the lack of symmetries in general curved space times, it is simply not possible to fix a particular vacuum state. Since one is free to choose a coordinate system, it is impossible by principle to have a physically unambiguously preferred vacuum. As mentioned above, there are however situations in which one can relate the states of one representation with the states of

another representation. In many cases, this fails namely when the mean density of one particle species, in the other vacuum is infinite. This problem will also occur in the quantum field theories we have in mind, and we will come back to this issue in chapters 4, 8 and 9.

2.2.8. Power Spectrum

Coming back to the standard cosmological model starting with the semiclassical picture of cosmological quantum perturbations on a classical homogeneous background, it is generically assumed that these perturbations are stretched during the cosmic expansion and evolve into today's large scale structure. During this process, the perturbations become classical, possibly by a process of decoherence. In order to compare the theoretically predicted scalar perturbations that obey the above equations of motion with observations, it is necessary to compute a statistically relevant measure of these perturbations as it is impossible to trace back the exact evolution of the perturbations starting with some specific initial conditions. A well–suited and simple tool are the power spectra of the scalar (and tensor) perturbations (Durrer 2008; Piattella 2018), that directly depend on the mode amplitudes v_k of the perturbations. In case of Gaussian random fluctuations, this statistical measure is indeed sufficient to reproduce all the statistical information contained within the perturbative fields (it relies on computing the two–point functions). The power spectrum is given by (Baumann 2012)

$$\Delta_v^2(k) = \frac{k^3}{2\pi^2}|v_k|^2, \tag{2.53}$$

and the amplitude of the modes v_k is to be extracted at the end of inflation. The initial conditions for the quantum fields are set at the beginning of inflation at which point the Universe is expected to be in an almost de Sitter state. Moreover, at sufficiently early times, all modes of cosmological interest are presumably well inside the cosmological horizon, i.e., $k^2 \gg \zeta''/\zeta$. One can hence disregard the time–dependent potential term in the mode equations of motion, which gives rise to a quantum field in Minkowski space time. Consequently, the cosmological paradigm sets Minkowski initial conditions for the perturbative fields which give rise to a unique and well–defined vacuum state. These initial conditions are then evolved according to a simplified mode equation of motion in de Sitter space (the modes can leave the horizon during inflation).

The mode amplitudes at the end of inflation then serve to compute the primordial power spectrum. This spectrum in turn gives the initial conditions for the equations of motion that govern the evolution of the cosmological perturbation during its later history up to the present date. The evolution underlies a coupled set of Boltzmann equations of the different matter species present during the various stages of the cosmic history. Analytical investigations of this evolution are too complex but there are a range of cosmological numerical codes that allow to trace the evolution of the matter species during these times, e.g., the Cosmic Linear Anisotropy Solving System (CLASS) (Blas, Lesgourgues, and Tram 2011; Lesgourgues 2011). These codes generate the late–time angular power spectrum that can be compared to the observable traces of, for example the CMB Temperature anisotropies (or rather its two point correlators), see Figure 2.2.

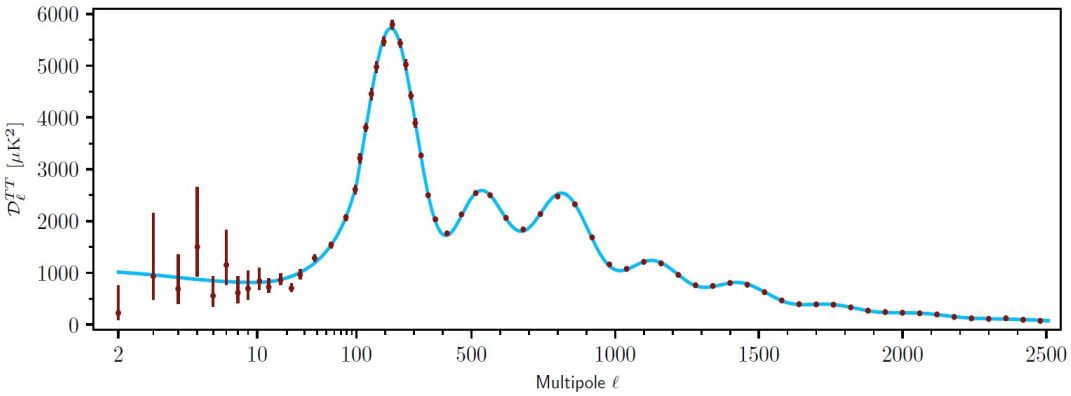

Figure 2.2.: Planck CMB foreground–subtracted angular power spectrum for temperature, taken from (Aghanim et al. 2020a). The blue lines show the best–fitting standard ΛCDM model.

2.3. Problems and Inconsistencies

In the following section, we examine the open questions and problems inherent to the standard concordance cosmological model as outlined before. We note that this section coincides in large parts with segments of reference (Schander and Thiemann 2021).

The ΛCDM concordance model based on the pillars of the Standard Model of particle physics and general relativity has shaped our current view of the Universe, and has been the driving force behind many of the breakthroughs of modern cosmology, for example the prediction and the discovery of the CMB radiation (Aghanim et al. 2020a,b; Alpher and Herman 1948a,b; Gamov 1948a,b; Penzias and Wilson 1965). Modelled by only six parameters (Aghanim et al. 2020b; Spergel 2015), it features an impressive simplicity while correctly predicting and fitting large parts of the existing cosmological data (Aghanim et al. 2020a,b).

As we have seen, one of the most important assumptions within the ΛCDM paradigm is that the Universe is almost spatially homogeneous and isotropic in a statistical sense. Within the standard ΛCDM model, small inhomogeneities on any scale smaller than the observable Universe are presumed to evolve following the underlying FLRW background structure, but conversely their presence does *not* affect the global FLRW evolution. More precisely, it is assumed that effects from the small scale inhomogeneities onto the largest scales can be neglegted, i.e., there is no substantial backreaction.

Doubts regarding the simplistic nature and the question of backreaction have gained momentum in recent years. In fact, the ΛCDM model, as appealing it may be, leads to the conclusion that approximately 69% of the energy budget of our Universe consists of a yet unknown fluid, dubbed “dark energy” (Aghanim et al. 2020b), and which drives the very recent accelerated expansion of the Universe (Peebles and Ratra 2003; Perlmutter et al. 1999; Riess et al. 1998). Most of the remaining 31% of the energy budget is credited to another yet unknown form of cold “dark” matter (Aghanim et al. 2020b; Blumenthal et al. 1984; Peebles 1982) which provides an explanation for the characteristic rotation and motion of the remaining 6% of ordinary matter in the Universe. In summary, we are faced with the problem that we are literally in the dark about 94%

of the energy and matter content of the observable Universe.

We emphasize that the creativity of researchers in terms of possible solutions to these two problems seems almost inexhaustible. On the dark matter front, weakly interacting massive particles (WIMPs) are among the most famous candidates but none of the proposed solutions could yet be detected (Bertone and Hooper 2018). Another proposal is that dark matter is constituted (partly) by primordial black holes (Carr and Kühnel 2020; Carr, Kühnel, and Visinelli 2020). Regarding dark energy, the simplest explanation could be a fundamental energy of space apparent through the cosmological constant Λ while for example the existence of an additional dynamical field (the "quintessence") would provide another answer (Ratra and Peebles 1988). But long story short – we still don't know the answer.

In recent years, these conceptual problems have been accompanied by tensions in the estimates of certain cosmological parameters as made by different collaborations (Di Valentino et al. 2021a,c; Pesce et al. 2020). The evaluation of the Hubble constant H_0 as performed by the Planck collaboration (explicitely assuming a ΛCDM model) gives a value of $H_0 = (67.27 \pm 0.60)\mathrm{km}/(\mathrm{s} \cdot \mathrm{Mpc})$ (Aghanim et al. 2020b) while the SH0ES collaboration finds $H_0 = (74.03 \pm 1.42)\mathrm{km}/(\mathrm{s} \cdot \mathrm{Mpc})$ (Riess et al. 2019) which in turn is based on the measurements of the Hubble Space Telescope, see also Figure 2.3. This leads to a tension at the 4.4σ–level (Di Valentino et al. 2021c). While others (Efstathiou 2020; Freedman 2021) claim that this tension can be alleviated by a careful analysis of the late time cosmological measurements, there is no consensus within the research community about this question.

Furthermore, the estimate of the parameter S_8, a measure for the matter energy density Ω_m and the amplitue of structure growth σ_8, is subject to similar but less stringent discrepancies (see Figure 2.3). Its value as determined by the Planck collaboration (Aghanim et al. 2020b) and other low–redshift measurements (Heymans et al. 2020) is in tension above the 2σ – level (Di Valentino et al. 2021a). There are also numerous proposed solutions for this problem, some of them adding further content to the model of the early Universe (Di Valentino, Mena, et al. 2021), others claim that the systematic uncertainties related to the Cepheid color–luminosity calibration prevents us from correctly measuring H_0 at late times (Mortsell et al. 2021). Interestingly, Krishnan et al. (2021) propose that the Hubble tension indicates a possible breakdown of the FLRW model and possibly the assumption of an isotropic Universe.

Indeed, it has been claimed, inspired by the work of Ellis and Baldwin (1984) that even the assumption of the cosmological principle should be questioned according to the evaluation of measurement data of the preliminary CatWISE quasar catalogue (Eisenhardt et al. 2020). More precisely, Secrest et al. (2021) assert that our peculiar velocity with respect to these quasars is different from the peculiar velocity of the CMB, and hence the kinematic interpretation of the CMB dipole is rejected with a p–value of 5×10^{-7}, or put otherwise, is in 4.9σ tension with observations. Similar conclusions were already drawn by Colin et al. (2011). On the other hand, Stahl et al. (2021) find results inferred from measurements of recent supernovae of types Ia and II consistent with the Planck results and the ΛCDM model.

Furthermore, in (Bullock and Boylan–Kolchin 2017; Del Popolo and Le Delliou 2017), it is argued that the concordance model comprises also severe problems on the smallest scales which are reflected in discrepancies between the ΛCDM model and observations. For example, the cores

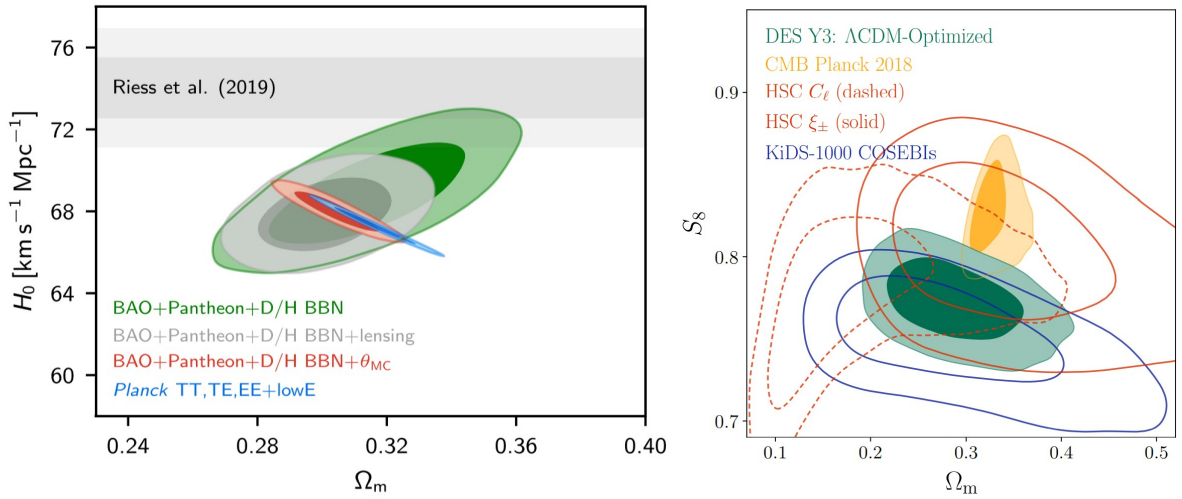

Figure 2.3.: Left panel: Inverse–distance–ladder constraints on the Hubble parameter and Ω_m due to (Riess et al. 2019) (grey bands), compared to the result from Planck (blue) (Aghanim et al. 2020b). Contours contain 68% and 95% of the probability. The figure is taken from (Aghanim et al. 2020a) where more details are given. Right panel: Cosmic shear results with constraints on S_8 and Ω_m for the Dark Energy Survey (DES Y3) (green) (Amon et al. 2021), the Planck 2018 CMB data (Aghanim et al. 2020c), (yellow), as well as the KiDS–1000 COSEBIs analysis (blue) and the HSC results (red). The figure is taken from (Amon et al. 2021), see also there for more references and explanations.

of many dark matter dominated galaxies are less dense and cuspy than predicted by the ΛCDM paradigm.

These pressing open questions on the observational side and the growing tensions between different parameter estimates indicate that there might be some fundamental problems in our understanding of modern cosmology and the theoretical models underlying it. Indeed, the criticism of many aspects of the ΛCDM model is growing louder in recent years. Many of the objections concern the inflationary paradigm that was introduced to solve some of the initial problems of the standard cosmological model. In particular, inflation was introduced to solve the monopole, the flatness and the horizon problem. Regarding the monopoles, one could however argue that there are simply no monopoles – in fact, we do not have observational evidence for a process that produces a high abundance of monopoles at earliest times. Hence, a natural proposal for explaining the non–existence of monopoles in the Universe is simply to assume that there haven't been any in the first place.

Regarding the fine tuning problems, one could argue that our discomfort to assume a very tiny value for the curvature density at earliest times is rather an aesthetic problem than a physical one. Nature could simply choose a large range of initial conditions – why should all the cosmological parameters be close to one? Finally, it is often claimed that inflation solves the problem of initial conditions in the sense that it provides a natural explanation for why our Universe has been almost homogeneous and isotropic throughout its history (the horizon problem). While inflation provides indeed a formalism for having causally connected patches in all directions of the sky at earliest times, it certainly does not ease the fine–tuning problem. More precisely, one needs a very specific set of parameters within the inflationary model for obtaining a long enough lasting phase of inflation and for producing the right amplitudes of the scalar density power spectrum (Adams,

Freese, and Guth 1991; Ijjas and Steinhardt 2016).

Moreover, an analysis of the standard Liouville phase space measure for cosomological models shows that single field inflationary models with large numbers of inflation (e.g., $N \geq 60$) are exponentially suppressed (Gibbons and Turok 2008; Penrose 1989). This fact can be related to the requirement that inflation requires a long lasting phase of potential energy dominance which is hard to attain (Ijjas and Steinhardt 2016). Eventually, we mention that already according to the Planck 2015 data release, many of the inflationary scalar field models have been experimentally excluded. While the Gaussian nature of the CMB perturbations eliminates the rather complex inflationary models and favors the single field models, the Planck 2015 data disfavors the single field models (Ijjas and Steinhardt 2016).

In either case, none of the known Standard Model particles and fields seem to resemble the postulated inflationary field or to give a hint regarding its origin. The only yet detected scalar field currently included in the Standard Model is the Higgs boson but in order to provide a long enough lasting inflationary phase at early times, the field would be required to be non–minimally coupled to gravity (Bezrukov and Shaposhnikov 2008).

Another criticism that is raised regarding the standard cosmological model both without and with an inflationary phase concerns the inherent singularities predicted by the theory. In fact, classical general relativity presumes that for an expanding Universe filled with ordinary matter the Universe encounters a "Big Bang" singularity with infinite density when going backwards in time (Hawking 1966). Furthermore, Borde, Guth, and A. Vilenkin (2003) have shown that also inflationary Universes are past–incomplete, and thus encounter the same singularity issues. It is claimed that these singularities predict the theory's own breakdown and should be avoided.

Despite these criticisms and the existing data, the theory of inflation remains an active field of research. On the other hand, many new proposals suggest to replace the inflationary paradigm by other cosmic scenarios such as bouncing cosmologies (Brandenberger and Peter 2017; Cai 2014; Novello and Perez Bergliaffa 2008). A wide variety of such bouncing approaches are being pursued, some of them are motivated by purely classical theories, e.g., (Ijjas and Steinhardt 2019) while others rely on quantum mechanical approaches to the early Universe, e.g., (Ashtekar, Pawlowski, and P. Singh 2006a).

While these approaches attempt to replace the almost homogeneous and isotropic inflationary paradigm using a variety of different approaches, most of them adhere to linear cosmological perturbation theory assuming that the test field perturbations propagate on a fixed (possibly quantum) cosmological background. In these models, the perturbations do not backreact on the cosmological homogeneous degrees of freedom, i.e., they do not alter the global evolution of the Universe. Such possible backreaction effects are neglected in most of the cosmological approaches, both for models of the late time Universe as well as for the early Universe. In view of the existing data situation and the growing discrepancies within the cosmological standard model, it seems however very timely to reassess the question of backreaction. Furthermore, as the H_0–tension might point to discrepancies of our concordance model in the very early Universe, it is important to further examine and understand theories of quantum gravity – of course coupled to matter. As explained in the introduction, a particularly interesting endeavor would be to consider the semi-classical limit of a quantum cosmological scenario (i.e., finding a QFT on a cosmological CST),

or more generically, to find (approximate) quantum solutions within such a theory of quantum cosmology with quantum matter. This requires an understanding of the inter–and backreaction of such quantum models.

Hence, in our view the question of backreaction is one of the most obvious and pressing ones as it examines not only one of the most important assumptions of modern cosmology (i.e., that cosmological backreaction can be neglected) but it also allows to approach the true quantum solutions of coupled gravity–matter systems. To investigate this question, no exotic new physics is needed (in the first place) but only the appropriate mathematical tools. The formalism employed to study this question in this thesis will also provide the means to analyze the semiclassical limit of such theories.

Therefore, in chapter 3 we first review the existing approaches to the problem of backreaction for the late time classical Universe. Chapter 4 examines the question of backreaction in semiclassical approaches to cosmology. In chapter 5, we revise the existing approaches to including backreaction in quantum mechanical approaches to cosmology. The remainder of this thesis will focus on one specific and new proposal for including purely quantum mechanical backreaction which relies on a very flexible and suitable formalism relying on the Born–Oppenheimer approach, and which we adapt for an application to quantum cosmological perturbation theory.

3. Classical Cosmological Backreaction

The previous chapter has underlined that the concordance ΛCDM model, despite its achievements, comes with many (often unstated) assumptions. One of them is the conjecture that cosmological backreaction is negligible, i.e., the assumption that any phenomenon related to the effects of cosmological inhomogeneities on the global or macroscopic evolution of the Universe can be ignored. In this chapter, we analyze the underlying problems that could arise due to neglecting such backreaction in purely classical approaches to cosmology, and provide an overview of the ideas discussed in the literature.

The topic is of course multifaceted and includes various aspects that require different methods and answers. An analysis of all the proposed approaches is beyond the scope of this work, and we therefore focus on the most relevant and most discussed ideas. Owing to the different physical situations, it is useful to distinguish between backreaction that occurs in the early and the late time Universe. Hereby, "late" refers to times after the decoupling of matter and radiation, whereas "early" studies encompass the inflationary Universe including the reheating phase. We start with a discussion of backreaction during the recent eras in cosmology and work our way back to the effects of backreaction in the early Universe. The former approaches rely on purely classical models of the late time Universe while some of the latter schemes (but not all) are based on quantum field theories on curved space times. The approaches based on quantum field theories will be the topic of the next chapter.

As far as it stands, there is no consensus on the question of backreaction, and results depend on the underlying physical model as well as on the averaging procedure being chosen. Our discussion of the late and early Universe backreaction effects in the following relies mainly on (but is not limited to the works by) Bolejko and Korzyński (2017), Clarkson, Ellis, et al. (2011), Ellis (2011), and Paranjape (2012), and references therein. A similar but shorter discussion of the topic can also be found in (Schander and Thiemann 2021), and certain parts of this paper coincide with parts of this section. The remainder of this thesis examines the question of backreaction in the *very* early Universe, where quantum effects for different parts of the cosmological system are presumed to play a role.

3.1. Backreaction in the Late Time Universe

To understand the issue of backreaction, it is useful to make a distinction between a truly spatially homogeneous and isotropic Universe, and a Universe which is only *statistically* homogeneous and isotropic (such as ours). In the first case, the geometric quantities of the theory as well as the matter content of the Universe reduce to FLRW form: the metric tensor can be parametrized by the scale factor $a(t)$ and the matter content may be described by a spatially homogeneous and

isotropic field or fluid. The Friedmann equations provide the corresponding equations of motion. In the case of a statistically homogeneous and isotropic Universe, there are inhomogeneities and obviously, the physical geometry and matter content fail to be well represented by an FLRW Universe. Nevertheless, it is reasonable to ask whether the ΛCDM model provides a good fit to the true lumpy Universe on its largest scales. This is the question underlying the "fitting problem" in cosmology (Ellis and Stoeger 1987), namely to define a suitable homogeneous and isotropic model with suitable cosmological parameters that fit well cosmological observations.

One possibility to make progress with regards to the fitting problem is to derive global quantities such as a global expansion parameter. For example, one could identify spatial hypersurfaces in space time and compute spatial volume averages of the local expansion rate. These averaged quantities however do *not* in general obey the Einstein equations (or the Friedmann equations) because the averaging process does not commute with evaluating the Einstein tensor (Ellis 2011). This is due to the non–linearity of Einstein's equations and can heuristically be understood as follows (Paranjape 2009): The Einstein tensor $G_{\mu\nu}[g]$ depends on derivatives of the Levi–Civita connection Γ associated with the metric as well as on its square Γ^2. Given an appropriate definition of spatial hypersurfaces in space time, an averaging over spatial volumes yields contributions $\langle\Gamma^2\rangle$ to the averaged Einstein equations while the matter content is described by the averaged stress–energy tensor $\langle T\rangle_{\mu\nu}$. In contrast, the Friedmann equations depart from the averaged metric tensor $\langle g\rangle$ and are assumed to have the form, $8\pi G\,\langle T\rangle_{\mu\nu} \equiv G[\langle g\rangle]_{\mu\nu} \sim \langle\Gamma\rangle^2_{\mu\nu}$. The first equality is hence an assumption! The true equations of motion valid on the averaging scale contain (a priori) non–vanishing contributions $E_{\mu\nu}$ of the form (Paranjape 2012)

$$G_{\mu\nu}[\langle g\rangle] = 8\pi G\,\langle T\rangle_{\mu\nu} + E_{\mu\nu} \sim 8\pi G\langle T\rangle_{\mu\nu} + \left(\langle\Gamma\rangle^2 - \langle\Gamma^2\rangle\right)_{\mu\nu} \tag{3.1}$$

where it was assumed that the Einstein equations hold for the inhomogeneous metric on the smallest scale where they have been excellently checked. The effects of backreaction have been stored into the additional effective stress–energy tensor $E_{\mu\nu}$.

The resulting equations and quantities obviously depend heavily on the concrete averaging procedure, the assumed matter content and on how inhomogeneities are built into the model. Likewise, the results range from negligible deviations from the assumed ΛCDM evolution to major changes of the theory such as works that aim at explaining the recent accelerated expansion of the Universe by backreaction (Buchert 2008; Heinesen and Buchert 2020).

The following sections provide a short overview of some of the relevant contributions, starting with approaches that focus on purely non–perturbative situations, then restricting to the manifestly perturbative methods, and continuing with an explicit consideration of numerical results. As advertised, we finish with an overview of classical backreaction in the early Universe.

3.1.1. Non–Perturbative Techniques

One possibility to quantify backreaction is to average a given inhomogeneous geometry and to compare the result to a purely homogeneous and isotropic solution to Einstein's equations. In a general relativistic setting, this problem was first considered by and, e.g., by considering the backreaction of gravitational waves on a slowly varying background (Ellis 2011). The seminal

work by Ellis (1984) transferred these ideas to cosmology, and in the sequel, many authors have proposed avenues to its solution among which Anastopoulos (2009), Carfora and Piotrkowska (1995), Futamase (1996), Kasai (1992), Mustapha et al. (1998), and Zotov and Stoeger (1992) in the non–perturbative regime (Paranjape 2009).

One challenge is to define a proper averaging mechanism for generic tensor fields since tensors at different space time points cannot simply be compared one to another in a curved background (Clarkson, Ellis, et al. 2011). A second issue is that a proper averaging procedure requires some information about the correct solution of geometry right from the beginning which is in most cases not available. In fact, one needs to choose physically reasonable spatial hypersurfaces to perform the averaging.

One of the most prominent approaches to a background independent averaging procedure was introduced by Buchert (2000, 2001), and is based on building spatial averages of scalar fields in inhomogeneous cosmologies. To illustrate the procedure, let us focus on late time cosmological situations using a pressureless vorticity–free dust as the matter content and comoving coordinates such that the equal–time hypersurfaces coincide with the matter rest frame. The gradient of the dust 4–velocity u^μ can be expressed in terms of the volume expansion rate θ and the shear tensor $\sigma_{\alpha\beta}$ using the decomposition (Buchert and Räsänen 2012)

$$\nabla_\beta u_\alpha =: \frac{1}{3} h_{\alpha\beta}\theta + \sigma_{\alpha\beta}. \tag{3.2}$$

The spatial average of a scalar field $S(t,x)$ over a spatial region D is defined with the induced spatial metric h as

$$\langle S\rangle_D(t) = \frac{1}{V_D}\int_D \mathrm{d}^3x\sqrt{h}\, S(t,x). \tag{3.3}$$

Since taking a time derivative does not commute with spatial averaging in this formalism (Clarkson, Ellis, et al. 2011) the averaging of the Einstein field equations yields an additional kinematical backreaction term $\mathcal{Q}_D$ in the Raychaudhuri equation for the volume scale factor $a_D \propto V_D^{1/3}$

$$3\frac{\ddot{a}_D}{a_D} + 4\pi G\,\langle\rho\rangle_D = \Lambda + \mathcal{Q}_D, \quad \mathcal{Q}_D := \frac{2}{3}\left[\langle\theta^2\rangle_D - \langle\theta\rangle_D^2\right] - 2\langle\sigma^2\rangle_D. \tag{3.4}$$

Note that structure formation and clustering in the late Universe lead to an increasing variance of the expansion rate, and hence to growing backreaction $\mathcal{Q}_D$ (Buchert and Räsänen 2012). If the backreaction acts similarly to a positive cosmological constant, as has been suggested by Nambu and Tanimoto (2005) and Räsänen (2004), this would yield a very natural solution to the coincidence problem, i.e., to the question of why the accelerated expansion starts just now when non–linear structure formation begins (Clarkson, Ellis, et al. 2011). To date, however, it is not clear as to which extent this formalism actually leads to observable predictions. Since the formalism only knows how to average scalar quantities, the resulting system of scalar equations is not closed and requires suitable external input to estimate the averaged shear (Ellis 2011). Consequently, backreaction can not be determined without ambiguity by this procedure.

Possible avenues to proceed are provided by the scaling solutions employed by Desgrange, Heinesen, and Buchert (2019), Larena et al. (2009), and Roy et al. (2011) which lead to results that can be compared to observations. In general, the averaged fields, e.g., the volume scale factor

do not have a clear physical meaning a priori (Clarkson, Ellis, et al. 2011). Räsänen (2009, 2010) argues however that they precisely describe observations along the past lightcone while Adamek, Clarkson, et al. (2019) underline that averaged quantities that are attached to the dust particles fail to provide a meaningful description of cosmological models when it comes to structure formation and shell–crossing. Instead, they advocate choosing averaging surfaces that correspond to the Poisson gauge as it results in negligible backreaction. Recently, Heinesen and Buchert (2020) have stressed that this approach lacks physical significance.

Another approach to the averaging problem which is manifestly covariant and hence eases the limitations of Buchert's formalism has been introduced by Zalaletdinov (2008). This scheme, denoted as "Macroscopic Gravity", relies on introducing an auxiliary so–called bi–local transport operator $\mathcal{A}^b_a(X,X')$ that acts as an integral kernel on a tensor $T_{ab}(X)$ in order to give its average $\bar{T}_{ab}(X)$ (Zalaletdinov 1997),

$$\bar{T}_{ab}(X) = \frac{\int_\Sigma d^4X' \mathcal{A}^{a'}_a(X,X')\mathcal{A}^{b'}_b(X,X')T_{a'b'}(X')}{\int_\Sigma d^4X\sqrt{|g|}}. \tag{3.5}$$

The transport operator $\mathcal{A}^b_a(X)$ is constructed such that its contractions with the actual physical operator transforms as a tensor at the point X but as a scalar elsewhere which allows to average over the space time region Σ (Clarkson, Ellis, et al. 2011). The field equations for the averaged quantities comprise an additional geometric correlation tensor that can be understood as an additional source term due to backreaction (Clarkson, Ellis, et al. 2011). In a flat FLRW macroscopic background, the resulting backreaction takes the form of an additional spatial curvature term (Hoogen 2009), and it was shown that the scheme reduces to Buchert's formalism in an appropriate limit (Paranjape and T. P. Singh 2007). Since the averaging procedure depends on the choice of the transport operator, the scheme lacks however predictive power and it is not clear how the choice of the transport operator affects the theory (Hoogen 2010).

One major criticism inherent to both presented formalisms is that they focus on deriving effective equations of motion for the averaged metric which by itself lacks a direct physical meaning. The averaged geometric quantities do not relate directly to physical observables (Clarkson, Ellis, et al. 2011): In particular, physical observables are related to light emission by some distant sources, for example the angular diameter distance or the redshift, and backreaction should be evaluated with respect to these observables. This can of course be overcome by imposing further physical assumptions that relate the results to observations.

Within Buchert's scheme, this has been done using the above–mentioned scaling solutions. Within the Macroscopic Gravity approach, Paranjape (2008) and Paranjape and T. P. Singh (2008) conclude that backreaction effects remain negligibly small both in the perturbative as well as in the non–linear regime of gravity. On the other hand, Coley (2009) and Räsänen (2009, 2010) derived effective cosmological equations of motion related to an averaging procedure on the past null cone. Another proposal for defining covariant light–cone averages was put forward by Gasperini et al. (2011), but the procedure requires dynamical equations of motion to relate variables at different times (Clarkson, Ellis, et al. 2011). See also in (Fanizza et al. 2020) for a more recent generalized proposal with a direct application to cosmological situations. It is in fact possible that inhomogeneities directly influence the measurement of cosmological parameters (Ellis 2011), for

example the redshift and its drift (Koksbang and Hannestad 2016) or area distances (Bertotti 1966; Ellis 2011). The relevance of these effects depends of course on the actual distribution of matter in our Universe (Ellis 2011). Recently, many proposals regarding the measurement of the redshift and its possible drift have been made in order to falsify the question of the backreaction problem (Heinesen 2021a,b; Koksbang 2019, 2020, 2021).

In addition to the question of a meaninigful averaging mechanism, the evaluation of backreaction also raises the question of how to design the underlying model of the Universe. The ΛCDM model uses a purely homogeneous and isotropic fluid to represent the matter content that drives the global evolution of the Universe. But the Universe is made up of structures and meta–structures that cluster in certain regions while other regions are almost empty. In the field of *Inhomogeneous Cosmology* (Bolejko, Celerier, and Krasinski 2011; Krasinski 2006) many proposals have been made to improve the simplistic assumptions of the standard model, some of which have been used to evaluate backreaction (Bolejko and Korzyński 2017; Clarkson, Ellis, et al. 2011).

One proposal by Wiltshire (2009) is the "Timescape Cosmology" which separates the Universe into underdense expanding regions bounded by overdense virialized structures. Wiltshire also computes an average using Buchert's formalism but it turns out that the strength of the corresponding backreaction is limited to a few percent (Clarkson, Ellis, et al. 2011). More importantly, the different time measures in the overdense regions and the averaged model have the effect of an additional redshift for observers in the overdense region which could account for the dimming of supernovae (Ellis 2011; Leith, Ng, and Wiltshire 2008). Similar attempts but with different assumptions for the matter distribution in the Universe are the Swiss Cheese model (Biswas and Notari 2008; Kantowski 1969; Tomita 2000), modifications of an FLRW Universe by introducing spherically symmetric Lemaître–Tolman–Bondi or Szekeres dust space times (Bolejko and Celerier 2010; Marra, Kolb, and Matarrese 2008).

All these models rely on introducing a cosmological fluid that is consistently modified, but the matching conditions assure that the global evolution of the models do not differ from the standard FLRW expansion (Clarkson, Ellis, et al. 2011). Inhomogeneous cosmologies that do not assume an underlying FLRW background are for example regular black hole lattices (e.g., (Yoo and Okawa 2014)) or the Lindquist–Wheeler models which consist of a regular lattice of Schwarzschild domains that are bounded by matter shells (Lindquist and Wheeler 1957). Interestingly, the global evolution in these models approximately follows the corresponding FLRW evolution (Clarkson, Ellis, et al. 2011). Although this restricts their value for evaluating backreaction as an effect on the global evolution of the Universe, they provide insights into backreaction effects on light propagation (Krasinski and Bolejko 2011; Sussman 2011).

In summary, we acknowledge that evaluating the form and strength of backreaction for non–perturbative inhomogeneous cosmology is a difficult task. There are several proposals for how to average the inhomogeneous fields in order to obtain macroscopic quantities that one can compare with global cosmological parameters. All presented schemes require to make a priori assumptions that have physical consequences, for example the choice of a suitable averaging volume or the form of the bi–local transport operator in Macroscopic Gravity. There is no consensus regarding these questions so far. One possibility to yet make progress is to construct a viable model of the Universe that admits exact solutions and to compare its evolution and observable quantities with an assumed FLRW Universe. This comes however at the price of oversimplifying the true lumpy

Universe and care must be taken in the choice of boundary and matching conditions (Bolejko and Korzyński 2017). It is thus of interest to analyze perturbative FLRW based models whose results on backreaction effects can possibly be compared to cosmological observations without ambiguities owing to the theoretical framework (Clarkson, Ellis, et al. 2011). Of course, it must be noted that this approach might not be adequate during recent times when structures have formed. These computations for backreaction need a particular FLRW background solution as an input. But this background will be altered by the effects of backreaction. We can thus never start with the correct background — a vicious circle (Paranjape 2009).

3.1.2. Perturbative Techniques

Perturbative models assume that the Universe is well described by a spatially homogeneous and isotropic solution to Einstein's equations with small perturbations. The question is thus whether and to which extent the perturbative fields alter the dynamics of the homogeneous background solution in a linear or weakly non–linear regime. The goal of the game is to compute averaged macroscopic quantities which include backreactions by the perturbations and which can ultimately be compared to observable quantities such as the luminosity distance.

Similar to the non–linear regime, the explicit backreaction effect depends on the chosen averaging scheme and the underlying matter model. The results of the averaging formalisms by Buchert and Zalaletdinov, although constructed for explicitely non–perturbative models, can be applied to the perturbative cosmological regime. This has for example been done by Paranjape and T. P. Singh (2007) for Macroscopic Gravity and the Buchert scheme, the result being negligible backreaction effects in the new effective Friedmann equations. Other proposals for averaging schemes that explicitely apply to the perturbative regime were proposed by Boersma (1998), Futamase (1996), and Noonan (1984), see also (Paranjape 2009).

Most of the works tie in with cosmological observations and consider flat ΛCDM models with Gaussian scalar perturbations to start with (Ellis 2011). To evaluate backreaction, they compute the deviations to the Hubble expansion rate or similar variables that are caused by backreaction (Clarkson, Ananda, and Larena 2009; Clarkson and Umeh 2011; Kolb, Marra, and Matarrese 2010; Kolb, Matarrese, Notari, et al. 2005; N. Li and Schwarz 2008; Russ et al. 1997), or give effective Friedmann equations with additional contributions (Baumann et al. 2012; Behrend, I. Brown, and Robbers 2008; I. Brown, Robbers, and Behrend 2009; Noonan 1984; Paranjape and T. P. Singh 2007; Peebles 2010), see also (Clarkson, Ellis, et al. 2011).

The basic idea underlying the perturbative treatments is to expand the metric and the matter fields in first (and second) order perturbation theory and to write the deviations of the original theory in terms of averages of these perturbative fields. The assumption is hence that the real inhomogeneous Universe, consisting of large voids between the matter dominated regions, can be well described using a Newtonian approximation (Ellis 2011). This conjecture has been supported for example by Baumann et al. (2012) and Ishibashi and Wald (2006). In fact, Buchert, Ellis, and Elst (2009) estimate the relative size of spatial metric perturbations at the scale of voids and walls in our Universe to be of the order of 10^{-5}, and which would hence support the perturbative ansatz. The field equations include however density perturbations of the form $k^2\delta g$ where k is the mode number of the field and which can be large (Clarkson, Ellis, et al. 2011).

To evaluate the corrected global Hubble expansion rate, it is convenient to first compute a spatial average over some appropriate macroscopic domain (like for the non–perturbative approaches above), and to use then the given statistical information about the perturbation fields in guise of their power spectra in order to give concrete estimates of the size of the effects (Clarkson, Ellis, et al. 2011): More precisely, one computes the corresponding ensemble average of, for example the Hubble rate, including second order terms due to the perturbations. First order terms in the metric perturbations drop out (that is why a second order extension is needed), and one is left with computing the ensemble averages of the spatial averages $\langle \partial^m \Phi \partial^n \Phi \rangle$, $n, m \in \mathbb{N}$, as far as the Hubble expansion rate is concerned. Here, Φ denotes the Newtonian potential of the metric which is perturbed using a Poisson gauge.

Employing the observational constraints on the power spectra, it turns out that the dominant contributions are at most of the order of 10^{-5} which is due to the large horizon scale at matter equality, or equivalently, the low temperatures at that time, and backreaction only depends on the modes that are larger than this scale (Clarkson, Ellis, et al. 2011). The subdominant terms depend directly on an IR–cutoff that is necessary for the computations and which is set by the largest modes we can observe today. It reflects our ignorance of physics that might happen on larger scales, and some have claimed that this could result in observable backreaction effects (Clarkson, Ellis, et al. 2011), namely by finding a bound for the start of inflation which basically determines the cutoff (Barausse, Matarrese, and Riotto 2005; Kolb, Matarrese, Notari, et al. 2005; Kolb, Matarrese, and Riotto 2006) while others disagree in this respect (Flanagan 2005; Geshnizjani, Chung, and Afshordi 2005; Hirata and Seljak 2005).

Regarding the corrections to the variance of the Hubble rate and the deceleration parameter $q = -(1 + \dot{H}/H^2)$, the second order perturbative contributions include averaging terms that manifestly depend on an artificial UV–cutoff which should in principle be set by the end of inflation and the structure scale of dark matter (Clarkson, Ellis, et al. 2011). And even if the cutoff is set by larger scales (i.e., larger than the scales of non–linearity), it can lead to large backreaction of order unity in the variance of the Hubble rate, see also in the previous reference. Baumann et al. (2012) propose a reformulation of perturbation theory which could ease the problem. More precisely, they develop an effective field theory valid on large scales $k \ll \Lambda$ while carefully implementing a split of long and short wavelength modes in their effective equations of motion. They find no significant backreaction on the largest scales but claim that there are relevant effects on the baryon accoustic oscillations. This promising approach has however been critizised to neglect backreaction terms due to their partly non–Riemannian averaging procedure (Clarkson, Ellis, et al. 2011).

The problems that arise for Riemannian averaging have been addressed by Green and Wald (2011, 2012, 2013) using a weak field limit. Instead of considering averages of inhomogeneous fields over a certain volume as discussed above, they define a point limit process for the cosmological inhomogeneities. They find that backreaction for matter that behaves non–relativistically on small scales can only occur in form of an effective radiation stress–energy tensor, and they claim that the overal FLRW evolution is not significantly affected by such backreaction (Green and Wald 2014). Their scheme omits however the effects of matter clustering (which should be the most relevant contribution to backreaction) (Ellis 2011), and it has been questioned whether the limiting process can describe any realistic situation in nature (Buchert et al. 2015).

This last criticism seems to be inherent to any of the discussed approaches that consider averaging over spatial or spatio–temporal volume cells. What is however being measured are quantities that are related to light emission (such as the redshift and the angular diameter distance), and one could ask whether a null–fitting, i.e., an averaging procedure along the past null cone, yields meaningful results (Clarkson, Ellis, et al. 2011). The ideas for how this might work in a perturbative setting were laid out in a seminal work by Kristian and Sachs (1966). These ideas were for example used by Flanagan (2005) to compute the deceleration parameter as measured by comoving observers. Other approaches evaluate the effects of perturbations on observable quantities such as the distance–redshift relation (Barausse, Matarrese, and Riotto 2005; Bonvin, Durrer, and Gasparini 2006) which includes corrections as the ones to the Hubble rate. Second order (possibly large) contributions might furthermore affect the variance of the luminosity distance average as well as the deceleration parameter (Clarkson, Ellis, et al. 2011).

Finally, it is fair to say that there is no consensus on the question of backreaction in perturbative cosmology. It is however clear that the Newtonian potential, responsible for the backreaction in many of the approaches, is very small (except in the vicinity of heavy objects such as neutron stars) and the peculiar form of its power spectrum (namely its small magnitude on large scales) prevent the backreaction effect for any quantity that depends on Φ and its derivatives to be large (Clarkson, Ellis, et al. 2011). Only the variance of cosmological parameters might receive relevant backreaction effects but solely on small scales of a few Mpc. In general, it is not surprising that in a model for which the background is already fixed up to tiny perturbations the backreaction effects remain small, but it is of course questionable whether this approach is able to describe the physical reality in a very lumpy Universe (Ellis 2011). The sceptic will also oppose that backreaction is an effect due to full general relativity and cannot be captured with Newtonian approximations. Another open issue is whether higher order perturbation theory might change the given results, and as mentioned above, whether the ambiguities introduced by the IR– and UV–cutoffs play a role for the ultimate results (Clarkson, Ellis, et al. 2011).

3.1.3. Relativistic Simulations

Numerical methods for simulating the evolution of realistic relativistic space times might help to make progress on the question of backreaction, in particular in situations where exact solutions to Einstein's equations are out of reach. As it currently stands, several different coding environments are available (Bolejko and Korzyński 2017): The most important ones are the cosmological N–body code "gevolution" which includes relativistic effects by means of a weak field approximation (Adamek, Daverio, et al. 2016); the N–body code "GRAMSES" implementing a constrained formulation of general relativity (Barrera – Hinojosa and B. Li 2020); the numerical relativity "Einstein toolkit" based on the Cactus infrastructure (Loffler et al. 2012); and the numerical relativity code "Cosmograph" (Mertens, Giblin, and Starkman 2016) (for a comparison of the codes see Adamek, Barrera – Hinojosa, et al. 2020).

As an application to an inhomogeneous cosmological situation in which the matter content is modelled by a pressureless fluid, Mertens, Giblin, and Starkman (2016) employ the "Cosmograph" code and compare their simulation to the evolution of a homogeneous FLRW model. They show that inhomogeneities generate fluctuations in the extrinsic curvature parameter but defer

the evaluation of physical observables to future work. As another more concrete application to the backreaction problem, Bentivegna and Bruni (2016) use the Einstein toolkit in an Einstein – de Sitter Universe with small initial density perturbations in order to show that the kinematic backreaction term $\mathcal{Q}_D$ scales like $\frac{1}{a}$ but remains very small even for large perturbations. Also based on the Einstein toolkit, Macpherson, Price, and Lasky (2019) show that backreaction remains negligibly small in a CDM–Universe. All these results rely however on a fluid approximation which breaks down when it comes to structure formation and shell–crossing in the late time Universe.

In contrast, Adamek, Clarkson, et al. (2019) work with the gevolution code modelling a ΛCDM and an Einstein – de Sitter Universe with CDM–particles. Depending on the gauge – Poisson or comoving – and a corresponding choice of averaging hypersurfaces, they demonstrate that in the former case backreaction in the Hubble expansion rate remains always small (at the subpercent level), while when following the comoving dust particles, backreaction can become large ($\sim 15\%$). They subsequently argue that the correct question to ask is whether there are time slicings with respect to which backreaction remains small, while Heinesen and Buchert (2020) question the physical relevance of this hypothesis.

3.2. Backreaction in the Early Universe

For the evaluation of backreaction during the earliest cosmic eras, it seems admissible, according to the concordance model, to assume a spatially homogeneous and isotropic Universe with small perturbations. In line with the ΛCDM model, one can for instance assume an inflationary phase prior to the radiation dominated era and an FLRW metric plus perturbations to model the Universe as has been done for example by Abramo, Brandenberger, and Mukhanov (1997) and Mukhanov, Abramo, and Brandenberger (1997). We will explain the latter approach in more detail, and also review subsequent findings. Note that the following overview coincides with a section in (Schander and Thiemann 2021) which arose as a collaboration between T. Thiemann and the author.

The idea brought forward by Abramo, Brandenberger, and Mukhanov (1997) is to consider backreaction from long wavelength modes in models of the early Universe. Other earlier contributions in that direction were notably made by Tsamis and Woodard (1993, 1996). Their procedure improves on the strict perturbative truncation of the perturbative ΛCDM model by including second order contributions to the perturbative Einstein equations. Therefore recall from the previous chapter that in the standard perturbative treatment, the zeroth order homogeneous Einstein equations are assumed to hold exactly by neglecting any perturbations, i.e., $\Pi[\theta_0] = 0$. The evolution equations for the perturbations arise from considering any linear first–order terms of the field equations, namely $\Pi_{,a}[\theta_0]\delta\theta^a = 0$, together with the homogeneous solutions for θ_0 from the previous step.

A possible improvement of this truncation arises by performing a spatial average of the perturbative Einstein equations (2.40). Equipped with a global time parameter t and using that the spatial average of any perturbative field $\delta\theta^a$ vanishes, a set of improved Friedmann equations including backreaction effects up to second order can be derived (Abramo, Brandenberger, and

Mukhanov 1997):

$$\Pi[\theta_0] + \frac{1}{2}\left\langle \Pi_{,ab}\,[\theta_0]\delta\theta^a\,\delta\theta^b\right\rangle = 0. \tag{3.6}$$

Abramo, Brandenberger, and Mukhanov (1997) apply the scheme to an inflationary scalar field model with gauge–invariant cosmological perturbations, and consider the backreaction problem associated with an effective long wavelength energy momentum tensor. However, Unruh (1998) subsequently examined the question of whether this effect is indeed locally measurable, and found that such backreaction effects (in single field inflationary theories) can be absorbed by a gauge transformation (Abramo and Woodard 2002; Geshnizjani and Brandenberger 2002). It was then shown by Geshnizjani and Brandenberger (2005) that backreaction of such fluctuations becomes locally measurable after introducing an additional subdominant clock field, see also (Brandenberger and Lam 2004). This approach was then extended by Marozzi, G. Vacca, and Brandenberger (2013) based on the gauge–invariant formalism by Finelli, Marozzi, G. P. Vacca, et al. (2011). Besides, an extension of these works to second order perturbation theory shows that backreaction induced by super–Hubble perturbations is relevant even beyond perturbation theory and induces a negative contribution to the local Hubble expansion rate (Brandenberger, Graef, et al. 2018). Further contributions were notably made by Losic and Unruh (2005, 2008) who support the idea that backreaction represents a real and measurable effect in early Universe cosmology.

4. Quantum Field Theory on Curved Space Times

The considerations in the previous chapter were of a purely classical nature in that the gravitational as well as the matter fields were analyzed as classical fields. This seems to be a reasonable assumption for the late time Universe but it should be questioned for the earlier phases when the Universe was a hot and very dense place. In such situations, at least the matter degrees of freedom require a description with quantum field theoretical methods. The direct implementation of this idea leads to the wide terrain of quantum field theory on curved space times (QFT on CST) in which the quantum fluctuations of matter fields are coupled to a purely classical gravitational field. This should in fact provide a good approximation to physical situations where curved space time effects are significant, but the quantum nature of gravity is negligible. Due to its hybrid nature, it is clearly not a fundamental theory, but one can hope to make progress towards a more fundamental theory by asking the right questions within the approximative framework of QFT on CST.

The main issue of QFT on CST is to examine the structure of the quantum matter fields on some fixed curved space time determined by the classical gravitational field. Heuristically, this admits the picture of quantum fields propagating as test fields on a specific classical background, and the theory takes the effect of gravity upon the quantum fields into account. The backreaction effects of the quantum field fluctuations on the gravitational background are however neglegted in this framework. To include such backreaction, the approach of semiclassical gravity includes the expectation value of the quantum stress–energy tensor in some appropriate matter state as an effective source term in the Einstein equations, hence denoted as semiclassical Einstein equations. Another approach to including backreaction is denoted stochastic (semiclassical) gravity. In this framework, additional stochastic terms appear in the semiclassical Einstein equations.

Before attacking the question of backreaction in semiclassical (section 4.2) and stochastic gravity (section 4.3), we provide a review of the relevant notions and results of QFT on CST. The latter is based on (Birrell and Davies 1984; Hollands and Wald 2015; Wald 1995).

4.1. Quantum Field Theory on Curved Space Times

4.1.1. Covariant Approach

As the name suggests, *quantum field theory on curved space times* aims at defining a consistent quantum theory for (matter) fields that are coupled to a generic classical gravitational field. This is in fact not a trivial task since many of the fundamental concepts of QFT on Minkowski space time such as Poincaré invariance, and hence the notion of a Poincaré invariant vacuum state and excitations thereof are meaningless. Nevertheless, it is possible to define a set of basic principles,

inspired by Minkowski QFT, but which are more general in nature. These are as follows (Hollands and Wald 2015):

First, any quantum field $\mathbf{\Phi}$ is to be considered as a distribution on some space of test functions on the underlying Riemannian space time manifold $(\mathcal{M}, g)$ with metric tensor g, and with values in a quantum algebra $\mathcal{A}_Q = \mathcal{A}_Q(\mathcal{M}, g)$. The focus on the algebraic character releaves us from fixing one particular field representation. In fact, due to the infinite number of degrees of freedom, different representations of the field algebra are in general not unitarily equivalent – the Stone–von Neumann theorem does not apply here – and hence, the choice of a representation does not seem to be fundamental for the definition of a QFT on CST. We thereby follow the algebraic approach to QFT (Haag 1955). Second, the QFT should be locally and covariantly constructed, in the sense that information propagates according to the laws of general relativity and the fields should be constructed without any further background structure. Third, the fields of the QFT should obey a suitable so–called microlocal spectrum condition which translates the requirement of positive energy from QFT on Minkowski space time to the generic relativistic case.

With these preliminaries in mind, we give the basic notions and ideas of (algebraic) QFT on CST for a free real–valued scalar field $\Phi : \mathcal{M} \to \mathbb{R}$. The section is mainly based on (Birrell and Davies 1984; Hollands and Wald 2015). The classical Klein–Gordon field on a generically curved but globally hyperbolic space time $\mathcal{M}$ with Lorentzian–signature metric tensor g and generated by some smooth source $j : \mathcal{M} \to \mathbb{R}$ satisfies the equation of motion (Hollands and Wald 2015)

$$\left(g^{\mu\nu}\nabla_\mu\nabla_\nu - m^2\right)\Phi = j \tag{4.1}$$

where ∇_μ is the covariant derivative associated with g, and $m \in \mathbb{R}$ the mass of the scalar field. After a $(3+1)$–split, any pair f_1, f_2 of smooth functions on a spatial hypersurface σ with unit normal n^μ determine a unique solution Φ to the Klein–Gordon equation with

$$\Phi|_\sigma = f_1, \;\; n^\mu\nabla_\mu\,\Phi|_\sigma = f_2. \tag{4.2}$$

The solutions Φ of such an initial value formulation depend continuously and causaly on the initial data f_1, f_2, and on the source j, see (Hollands and Wald 2015) for more details. It is common to define the advanced and retarded propagators $E^\pm$ of the Klein–Gordon field as functions on $C_0^\infty(\mathcal{M})$ or equivalently as distributional kernels on $\mathcal{M}\times\mathcal{M}$ such that formally

$$\left(g^{\mu\nu}\nabla_\mu\nabla_\nu - m^2\right)E^\pm(x,y) = \delta(x,y) \tag{4.3}$$

where the operator on the left hand side acts on the first variable in a distributional sense. It will also turn out to be useful to define the "commutator function" $E := E^+ - E^-$.

The QFT of the Klein–Gordon field is then most suitably constructed by introducing a "quantum" algebra of observables $\mathcal{A}_Q(\mathcal{M}, g)$ that reflects the properties of the linear and real–valued Klein–Gordon field in an appropriate sense. Let therefore $\mathcal{A}_Q$ be a unital $*$–algebra with the involution $*$. A quantum field $\mathbf{\Phi} \in \mathcal{A}_Q(\mathcal{M}, g)$ is a distribution over the Riemannian manifold $(\mathcal{M}, g)$ such that for any set of smearing functions $f, f_1, f_2 \in C_0^\infty(\mathcal{M})$, the field $\mathbf{\Phi}$ has values in the unital "quantum" $*$–algebra $\mathcal{A}_Q$ and satisfies (Hollands and Wald 2015)

1. $\mathbf{\Phi}(c_1 f_1 + c_2 f_2) = c_1\mathbf{\Phi}(f_1) + c_2\mathbf{\Phi}(f_2)$, for all $c_1, c_2 \in \mathbb{C}$ (Linearity),

2. $\mathbf{\Phi}\left(\left(g^{\mu\nu}\nabla_\mu\nabla_\nu - m^2\right)f\right) = 0$ (Field equation),
3. $\mathbf{\Phi}(f)^* = \mathbf{\Phi}(\bar{f})$, (Hermicity),
4. $[\mathbf{\Phi}(f_1), \mathbf{\Phi}(f_2)] = iE(f_1, f_2)\mathbf{1}$ (Commutator relation)

where $\mathbf{1}$ is the one in the quantum algebra and an overbar denotes complex conjugation. Then, one can establish (Hollands and Wald 2015) that the linearity allows to informally interpret the field as an operator–valued distribution of the form

$$\mathbf{\Phi}(f) = \int_{\mathcal{M}} \mathrm{d}^4x\sqrt{g}\,\mathbf{\Phi}(x)f(x). \tag{4.4}$$

The notion of a physical state ω refers to a linear map $\omega : \mathcal{A}_Q \to \mathbb{C}$ which is normalized, $\omega(\mathbf{1}) = 1$, and positive, $\omega(\boldsymbol{A}^*\boldsymbol{A}) \geq 0$ for all $\boldsymbol{A} \in \mathcal{A}_Q$. By construction, any state is determined by the set of its n–point functions W_n with $n \geq 1$ defined by (Hollands and Wald 2015)

$$W_n(f_1, ..., f_n) := \omega(\mathbf{\Phi}(f_1)\cdots\mathbf{\Phi}(f_n)). \tag{4.5}$$

Given such a state or its n–point functions, we know all the expectation values of all powers of the field operators $\mathbf{\Phi}(f)$, and hence we have all physical information that can be extracted. Two states ω and ω' can be taken to form a new state via their convex linear combination $\lambda\omega + (1-\lambda)\omega'$ where $0 \leq \lambda \leq 1$. A state is called pure if it cannot be decomposed into a non–trivial convex linear combination.

There is also a direct relation between the algebraic states defined above and vector states in a Hilbert space $\mathcal{H}$ (Hollands and Wald 2015): For this, one needs a Hilbert space $\mathcal{H}$ with a dense domain $\mathcal{D} \subset \mathcal{H}$ and a $*$–algebra of linear operators $\mathcal{A}_Q \subset \mathcal{L}(\mathcal{D})$ on this dense domain. Then, the algebraic state ω_ψ arises from a non–zero vector ψ in $\mathcal{D}$ according to

$$\omega_\psi(\boldsymbol{A}) := \frac{\langle\psi, \boldsymbol{A}\psi\rangle}{\langle\psi, \psi\rangle} \tag{4.6}$$

where $\langle\cdot,\cdot\rangle$ is the inner product in $\mathcal{H}$, and $\boldsymbol{A} \in \mathcal{A}_Q$. On the other hand, any algebraic state ω gives rise to a Hilbert space $\mathcal{H}$ with invariant domain $\mathcal{D}$, a representation $\boldsymbol{\pi}$ of $\mathcal{A}_Q$ on $\mathcal{H}$ and a vector $\Omega \in \mathcal{D}$ such that (4.6) holds. This is known as the GNS construction in QFT (Gel'fand and Naimark 1943; Segal 1947), and which proves that the algebraic and the Hilbert space representations in quantum field theory are essentially equivalent. However, the Hilbert space representation obviously chooses one particular representation, in constrast to the algebraic ansatz which is hence more general.

In order to filter the physically relevant states off the large class of admissible states on $\mathcal{A}_Q$, one can impose a set of natural conditions on the states (Hollands and Wald 2015). One relevant class of states known as Hadamard states are constructed such that i) they control the high frequency modes of the field, in the sense that, ii) the singular structure of the n–point functions at short distances should not be worse than for the vacuum state in Minkowski, and iii) the singular structure of the n–point functions should be of "positive frequency type" (Hollands and Wald 2015). This can be most precisely phrased in terms of wave front sets (Radzikowski 1996a,b). As it turns out, the restriction to Hadamard states is necessary in order to define expectation values

of polynomials of the fields and its derivatives at the same space time point, hence, they assure that a covariant renormalization prescription can be defined for the stress–energy tensor. A class of Hadamard states exists on any globally hyperbolic space time (Fulling, Narcowich, and Wald 1981; Gérard and Wrochna 2014) which makes them particularly useful in QFT on CST.

A generalization of the class of Hadamard states yields the adiabatic vacuum states (Junker and Schrohe 2002), initially introduced by Parker (1969) in order to describe particle creation in an expanding FLRW Universe (note that this notion of adiabaticity has to be strictly distinguished from the notion of adiabaticity in the space *adiabatic* perturbation theory approach). When extended to generically curved space times, the class of adiabtic states contains the class of Hadamard states as these are adiabatic states of "infinite order" (Junker and Schrohe 2002). We already encountered the adiabatic states in chapter 2 where they were defined by introducing a WKB ansatz (2.52) for the mode solutions of the Klein–Gordon field. It was pointed out that these mode solutions are iteratively constructed with respect to an adiabatic perturbation parameter under the assumption that the geometry changes slowly. An infinite iteration of this type yields precisely a Hadamard state.

Another very important class of states are the so–called Gaussian or quasi–free states. These are defined by the requirement that their connected n–point functions (Hollands and Wald 2015)

$$W_n^{\mathrm{c}}(\boldsymbol{A}_1, \dots, \boldsymbol{A}_n) := \frac{\partial^n}{\partial t_1 \dots \partial t_n} \ln\left[\omega\left(e^{t_1 \boldsymbol{A}_1 \dots t_n \boldsymbol{A}_n}\right)\right], \quad \boldsymbol{A}_1, \dots, \boldsymbol{A}_n \in \mathcal{A}_Q \tag{4.7}$$

be vanishing for all $n > 2$, i.e., Gaussian states are completely determined by their one– and two–point functions W_1^{c} and W_2^{c}. Accordingly, a Gaussian state is positive iff for any $f \in C_0^\infty(\mathcal{M})$ the two–point function $W_2(f, \bar{f})$ is positive semidefinite, which gives rise to a large set of admissible Gaussian states useful for QFT on CST.

Most interestingly, a certain class of Gaussian states can be identified with a vacuum state in a Fock representation of $\mathcal{A}_Q(\mathcal{M}, g)$ (while other Gaussian states include KMS (temperature) states) (Hollands and Wald 2015). Therefore one uses the two point function W_2 associated with the Gaussian state ω to define an inner product on $C_0^\infty(\mathcal{M}, \mathbb{C})$ and to identify corresponding degenerate vectors. The factor space of $C_0^\infty(\mathcal{M}, \mathbb{C})$ divided by the degenerate vectors yields a subspace $\mathfrak{h}$ of complex valued smooth solutions to the Klein–Gordon equation which correspond to the positive frequency modes known from the standard Hilbert space representation (Hollands and Wald 2015). $\mathfrak{h}$ is most conveniently referred to as the one–particle Hilbert space. The corresponding symmetric bosonic Fock space $\mathcal{F}_{\mathrm{s}}(\mathfrak{h})$ is given by

$$\mathcal{F}_{\mathrm{s}}(\mathfrak{h}) = \mathbb{C} \oplus \bigoplus_{n \geq 1} (\mathfrak{h} \otimes_{\mathrm{s}} \cdots \otimes_{\mathrm{s}} \mathfrak{h})_n \tag{4.8}$$

where $\otimes_{\mathrm{s}}$ is the symmetrized tensor product, here applied n times. It is then convenient to choose a representation π of the quantum algebra $\mathcal{A}_Q$ given by

$$\pi\left[\boldsymbol{\Phi}(f)\right] = \boldsymbol{a}\left([f]\right)^* + \boldsymbol{a}\left([f]\right), \tag{4.9}$$

and we identify the usual creation and annihilation operators $\boldsymbol{a}^*([f]) \in \mathcal{L}(\mathcal{F}_{\mathrm{s}})$ and $\boldsymbol{a}([f]) \in \mathcal{L}(\mathcal{F}_{\mathrm{s}})$ associated with the equivalence class of f in $\mathfrak{h}$. The vacuum state $\Omega \in \mathcal{F}_{\mathrm{s}}(\mathfrak{h})$ indeed co-

incides with the algebraic Gaussian state ω through the GNS construction (Hollands and Wald 2015). Another way of defining pure Gaussian states uses a set of smooth, complex–valued mode functions $u_k(x)$ where the modes k belong to an appropriate measure space $(X, \mathrm{d}\mu)$, and any mode function satisfies the Klein–Gordon equation (4.1) with zero source. For every $f \in C_0^\infty(\mathcal{M}, \mathbb{R})$, one defines a map $Kf : X \to \mathbb{C}$ by (Hollands and Wald 2015)

$$Kf(k) = \int_{\mathcal{M}} \mathrm{d}^4x\sqrt{g}\, u_k(x) f(x), \tag{4.10}$$

and we assume that Kf is square–integrable over X and that the span of these functions is dense in $L^2(X, \mathrm{d}\mu)$. Besides, the mode functions should be complete with respect to the Klein–Gordon inner product on $(\mathcal{M}, g)$ in the sense that

$$Im\left[\langle Kf_1, Kf_2\rangle_{L^2(X)}\right] = \frac{1}{2}E(f_1, f_2), \quad \forall f_1, f_2 \in C_0^\infty(\mathcal{M}). \tag{4.11}$$

This yields indeed the two–point function of a Gaussian state defined as

$$W_2(x, y) = \int_X \mathrm{d}\mu(k) u_k(x)\overline{u}_k(y). \tag{4.12}$$

Since K is well–defined on the equivalence classes $[f]$ and provides a bounded isomorphism $K : \mathfrak{h} \to L^2(X, \mathrm{d}\mu)$, the GNS representation yields the symmetric Fock space $\mathcal{F}_s(L^2(X, \mathrm{d}\mu))$ as a Hilbert space and the representation π on this Fock space can be informally written as

$$\pi(\mathbf{\Phi}(x)) = \int_X \mathrm{d}\mu(k)\left[u_k(x)\,\boldsymbol{a}_k + \overline{u}_k(x)\,\boldsymbol{a}_k^*\right]. \tag{4.13}$$

From this, one recovers the standard Fock representation on Minkowski space if we identify the modes k with the wave vectors k in $\mathbb{R}^3$, and $u_k(x,t) = e^{-i\omega_k t + ikx}/\sqrt{2\omega_k}$. Considering the flat three–torus, as we will frequently do, k is in $\mathbb{Z}^3$ and we have the same mode functions.

In general, two representations $(\mathcal{H}, \pi, \Omega)$ and $(\mathcal{H}', \pi', \Omega')$ of the field algebra are said to be unitarily equivalent if there exists an isometry $U : \mathcal{H} \to \mathcal{H}'$ such that $U\pi(\boldsymbol{A})U^* = \pi'(\boldsymbol{A})$ for all $\boldsymbol{A} \in \mathcal{A}_Q$ (Hollands and Wald 2015). This means that two unitarily equivalent representations are physically equivalent in the sense that the physical results do not depend on the choice of the representation. It is hence an important question which of the representations of a field algebra can be identified as unitarily equivalent, and it turns out that most of the representations are not unitarily equivalent. In case of two Gaussian states ω and ω', a necessary condition for them to be unitarily equivalent is that there exists a constant c such that (Hollands and Wald 2015)

$$\frac{W_2(f,f)}{c} \leq W_2'(f,f) \leq c\, W_2(f,f), \quad \forall f \in C_0^\infty(\mathcal{M}, \mathbb{R}). \tag{4.14}$$

In fact, it is easy to construct states which violate this condition. Let us make this more explicit by using a mode decomposition, and for simplicity, let us assume that we are on the flat three–torus, and the modes k are hence in $\mathbb{Z}^3$. The representations of the two algebraic states are given by,

$$\pi(\mathbf{\Phi}(x)) = \sum_k \left[u_k(x)\,\boldsymbol{a}_k + \overline{u}_k(x)\,\boldsymbol{a}_k^*\right], \quad \pi'(\mathbf{\Phi}(x)) = \sum_{\vec{k}} \left[u_k'(x)\,\boldsymbol{a}_k' + \overline{u}_k'(x)\,\boldsymbol{a}_k'^*\right]. \tag{4.15}$$

As both sets of mode functions are required to be complete, it is possible to expand one set of mode functions in terms of the other set,

$$u'_k(x) = \sum_j \left[\alpha_{kj} u_j + \beta_{kj} \overline{u}_j\right]. \tag{4.16}$$

These are the well–known Bogoliubov transformations (Bogoliubov 1958) with the Bogoliubov coefficients α_{kj} and β_{kj}. They satisfy (Birrell and Davies 1984)

$$\sum_k \left[\alpha_{ik}\overline{\alpha}_{jk} - \beta_{ik}\overline{\beta}_{jk}\right] = \delta_{ij}, \quad \sum_k \left[\alpha_{ik}\beta_{jk} - \beta_{ik}\alpha_{jk}\right] = 0. \tag{4.17}$$

With that it is easy to show that the annihilation operators of the two representations are related according to

$$\boldsymbol{a}_k = \sum_j \left[\alpha_{jk}\, \boldsymbol{a}'_j + \overline{\beta}_{jk}\, \boldsymbol{a}'^*_j\right], \quad \boldsymbol{a}'_k = \sum_j \left[\overline{\alpha}_{jk}\, \boldsymbol{a}_j - \overline{\beta}_{jk}\, \boldsymbol{a}^*_j\right] \tag{4.18}$$

It is hence clear that non–vanishing $\beta'_{ij}s$ prevent the associated Fock spaces from being unitarily equivalent, in particular Ω' will in general not be annihilated by $\boldsymbol{a}_k$, i.e., $\boldsymbol{a}_k\Omega' \neq 0$. Even worse, one vacuum state may correspond to an infinite number of excitations with respect to the other representation. Therefore, let us consider the operator $\boldsymbol{N}_k := \boldsymbol{a}^*_k\boldsymbol{a}_k$ for the number of u_k–mode particles, and compute its expectation value with respect to the vacuum Ω'. This gives (Birrell and Davies 1984)

$$\langle\Omega', \boldsymbol{N}_k\, \Omega'\rangle_{\mathcal{H}'} = \sum_j \left|\beta_{kj}\right|^2. \tag{4.19}$$

Hence, if the right hand side of this equation is not finite, the vacuum state of the second representation carries infinitely many particles with respect to the first representation, and the two representations cannot be unitarily equivalent.

4.1.2. Hamiltonian Formalism

The above considerations of QFT on CST were presented in a covariant manner in the sense that no space time split was performed. Even if this proceeding best reflects the nature of the underlying concepts of general relativity, it is often useful to perform a split. It allows us to carry out a Hamiltonian analysis required for the following chapters. This section is mainly based on the textbooks by Fulling (1989), Peskin and Schroeder (1995), and Reed and Simon (1975b).

In Minkowski space, the relation between the covariant formalism and the standard Hamiltonian framework can be established by using only certain classes of smearing functions (Reed and Simon 1975b). In particular, the Hamilton formalism requires an initial value formulation in which the smearing fields have support on one precise spatial hypersurface. Formally, this can be achieved by using distributional smearing functions that are delta distributions with respect to time (i.e., they restrict the field to one spatial hypersurface) and ordinary test functions (for example Schwartz functions) with respect to the space coordinates. Unfortunately, smearing by a distribution is not an a priori well–defined procedure and one must assure that the given theory allows one to do so. However, if this is possible such a restriction gives in fact rise to the standard Hamiltonian quantum field theory. We refrain from going into more details as this is not relevant

for this thesis but refer the interested reader to the book by Reed and Simon (1975b, part X.7.).

We directly suppose that such a Hamiltonian formalism is available, and consider a Riemannian space time manifold $(\mathcal{M}, g)$ which is globally hyperbolic, $\mathcal{M} = \mathbb{R} \times \sigma$, and consequently admits a foliation into spatial hypersurfaces $\Sigma_t = \sigma$, labelled by the cosmic time parameter $t \in \mathbb{R}$. We consider the case of a spatially homogeneous and isotropic gravitational field with the scale factor a as its only dynamical degree of freedom. The classical action of a free Klein–Gordon scalar field with mass $m \in \mathbb{R}^+$ and coupling constant $\lambda \in \mathbb{R}^+$ on this geometry is given by (Fulling 1989)

$$S_\Phi[a, \Phi] = \frac{1}{2\lambda} \int_{\mathbb{R}\times\sigma} \mathrm{d}t\, \mathrm{d}^3x \sqrt{\tilde{h}^0}\, a^3 N \left(\frac{\dot{\Phi}^2}{N^2} - \frac{1}{a^2} \Phi \left(-\Delta + a^2 m^2 \right) \Phi \right) \tag{4.20}$$

where $\sqrt{\tilde{h}^0}$ is the spatial volume element and $\Delta := D_a D^a$ is the Laplace–Beltrami operator associated with σ. A dot denotes a derivative with respect to t and N is the homogeneous lapse. A standard Legendre transformation yields for the canonically conjugate momentum of Φ:

$$\Pi_\Phi := \frac{\partial \mathcal{L}}{\partial \dot{\Phi}} = \frac{\sqrt{\tilde{h}^0} a^3}{\lambda N} \dot{\Phi}. \tag{4.21}$$

The infinite dimensional phase space Γ of the theory is spanned by the fields (Φ, Π_Φ) for every fixed time t. In order to define the Poisson brackets in Γ, we use a set of suitable test (or smearing) functions f_1, f_2, usually functions with compact support in (a chart of) the spatial manifold σ such that

$$\{\Phi(f_1), \Pi_\Phi(f_2)\} = \langle f_1, f_2 \rangle \tag{4.22}$$

is the only non–vanishing Poisson bracket. The angular brackets denote the inner product within the space of test functions. The Legendre transformation yields the Hamiltonian of the classical theory

$$H = \frac{1}{2\lambda} \int_\sigma \mathrm{d}^3x \sqrt{\tilde{h}^0}\, a^3 N \left(\frac{\lambda^2 \Pi_\Phi^2}{\tilde{h}^0 a^6} + \frac{1}{a^2} \Phi \left(-\Delta + a^2 m^2 \right) \Phi \right). \tag{4.23}$$

Since N is a Lagrange multiplier, we can arbitrarily fix its value without affecting the theory, and we choose here $N \equiv 1$. Besides, in this section the value of the coupling constant λ is of no relevance, and so we fix it to $\lambda \equiv 1$. In addition, we assume that the spatial manifold is a compact and flat manifold, i.e., the three–torus $\mathbb{T}^3 = S^1 \times S^1 \times S^1$. We choose its sides to have lengths 1 in all three directions. Certainly, a more extended analysis for general spatial manifolds would be possible. But since this is not the very emphasis of this section, we choose a topology that is as simple as possible. With this, we formally write the Hamiltonian as a function of a as

$$H(a) := \frac{1}{2a^3} \int_{\mathbb{T}^3} \mathrm{d}^3x \, \left(\Pi_\Phi^2 + \Phi \left(-\Delta a^4 + a^6 m^2 \right) \Phi \right) \tag{4.24}$$

where the scale factor should be understood as an external parameter. Note that the metric of the flat three–torus is the standard Euclidean flat metric on the respective domain. Consequently, its determinant evaluates to 1. We define the a–dependent frequency operator $\omega(a)$ on the space of two–times differentiable functions on $\mathbb{T}^3$ as

$$\omega(a)^2(f) := \left(-\Delta a^4 + a^6 m^2 \right)(f), \quad \forall f \in C^2(\mathbb{T}^3). \tag{4.25}$$

The corresponding quantum theory of fields promotes the classical fields to operator–valued distributions $\mathbf{\Phi}(f_1)$ and $\mathbf{\Pi}_\Phi(f_2)$ which are defined, as before, on a suitable space of test functions (Reed and Simon 1975b). The theory is accordingly defined by the commutator relation

$$[\mathbf{\Phi}(f_1), \mathbf{\Pi}_\Phi(f_2)] = i\,\langle f_1, f_2\rangle\,\mathbf{1} \tag{4.26}$$

where $\mathbf{1}$ is the one in the quantum operator algebra $\mathcal{A}_Q$. This commutation relation is compatible and actually follows from the commutator relation of the scalar field in section 4.1 after restricting to the above–mentioned appropriate class of smearing functions (Reed and Simon 1975b). A representation $\pi : \mathcal{A}_Q \to \mathcal{B}(\mathcal{H})$ of the field algebra on a suitable Hilbert space $\mathcal{H}$ in terms of (linear) annihilation and creation operators $\boldsymbol{b}(a,f) \in \mathcal{L}(\mathcal{H})$ and $\boldsymbol{b}^*(a,f) \in \mathcal{L}(\mathcal{H})$ can be given by (Hollands and Wald 2015)

$$\boldsymbol{b}(a,f) := \frac{1}{\sqrt{2}}\,\pi\left[\left(\sqrt{\omega(a)}\mathbf{\Phi}\right)(f) - i\left(\sqrt{\omega(a)}^{-1}\mathbf{\Pi}_\Phi\right)(f)\right], \tag{4.27}$$

$$\boldsymbol{b}^*(a,f) := \frac{1}{\sqrt{2}}\,\pi\left[\left(\sqrt{\omega(a)}\mathbf{\Phi}\right)(f) + i\left(\sqrt{\omega(a)}^{-1}\mathbf{\Pi}_\Phi\right)(f)\right], \tag{4.28}$$

for a suitable test function f. Here, the action of the operator $\sqrt{\omega(a)}$ on the quantum fields is to be understood in the distributional sense as $\sqrt{\omega(a)}\mathbf{\Phi}(f) := \mathbf{\Phi}(\sqrt{\omega(a)}f)$. By means of the commutation relation for the field operators, the commutator of the annihilation and creation operators are given by

$$[\,\boldsymbol{b}(a,f_1), \boldsymbol{b}^*(a,f_2)] = \langle f_1, f_2\rangle\,\mathbf{1}. \tag{4.29}$$

For any fixed value of a, the theory is very well–known and one can easily provide a concrete Hilbert space representation. For the time being, let therefore $a \equiv 1$ which precisely corresponds to the quantum Klein–Gordon field on Minkowski space. We omit any occurence of a and write

$$\omega^2(f) := \left(-\Delta + m^2\right)(f), \tag{4.30}$$

and introduce this operator ω into the formulae for the annihilation and creation operators $\boldsymbol{b}(f)$ and $\boldsymbol{b}^*(f)$. It follows that the field operators have the form

$$\pi\left[\mathbf{\Phi}(f)\right] = \frac{1}{\sqrt{2\omega}}\left(\boldsymbol{b}(f) + \boldsymbol{b}^*(f)\right), \quad \pi\left[\mathbf{\Pi}_\Phi(f)\right] = -i\sqrt{\frac{\omega}{2}}\left(\boldsymbol{b}(f) - \boldsymbol{b}^*(f)\right). \tag{4.31}$$

It is convenient to fix a basis of mode functions and to provide formulae for the annihilation and creation operators with respect to the label set of the basis. On the torus, we can consider the discrete mode functions

$$\{f_k(x) := \exp(-ikx)\}_k\,, \quad x \in [0,1]^3 = \mathbb{T}^3, \;\; k \in \Sigma := 2\pi\mathbb{Z}^3. \tag{4.32}$$

The mode functions f_k define a discrete basis for $L^2(\mathbb{T}^3, \mathrm{d}x)$, and most importantly are eigenfunctions of the Laplace operator on the torus such that $-\Delta f_k = k^2 f_k$. Hence, we also have that $\omega f_k = \sqrt{k^2+m^2}\,f_k$, and we consquently define $\omega_k := \sqrt{k^2+m^2}$. Due to the linearity of the fields and the completeness of the basis, we can expand the fields with respect to the modes and

define the mode annihilation and creation operators (Hollands and Wald 2015)

$$\boldsymbol{b}_k := \boldsymbol{b}(f_k) = \int_{\mathbb{T}^3} \mathrm{d}x\, \boldsymbol{b}(x) f_k(x), \quad \boldsymbol{b}_k := \boldsymbol{b}(f_k)^* = \int_{\mathbb{T}^3} \mathrm{d}x\, \boldsymbol{b}(x)^* f_k(x). \tag{4.33}$$

The hermicity of the canonical quantum fields imposes that $\boldsymbol{b}_{-k} = \boldsymbol{b}_k^*$. By expanding the Hamiltonian with respect to the mode functions, it follows that

$$\boldsymbol{H} = \frac{1}{2} \sum_{k \in \Sigma} \omega_k \boldsymbol{b}_k^* \boldsymbol{b}_k, \tag{4.34}$$

where we directly omitted the infinite vacuum energy contribution. It comes as no surprise that the annihilation and creation operators satisfy the standard commutation relations

$$\left[\boldsymbol{b}_k, \boldsymbol{b}_{k'}^*\right] = \delta_{k,k'} \mathbf{1}, \tag{4.35}$$

where $\delta_{k,k'}$ is now a Kronecker delta. An appropriate Hilbert space of this representation is the Fock space of some one particle Hilbert space $\mathcal{H}$ whose basis elements are labeled by the k–vectors. For example, we can use the mode basis $\{f_k\}$ on $L^2(\mathbb{T}^3, \mathrm{d}x) =: \mathcal{H}$. The corresponding symmetric Fock space is constructed according to (see the previous section)

$$\mathcal{F}_\mathrm{s}(\mathcal{H}) := \mathbb{C} \oplus \bigoplus_{n \geq 1} \left(\mathcal{H} \otimes_\mathrm{s} \cdots \otimes_\mathrm{s} \mathcal{H}\right)_n . \tag{4.36}$$

A symmetric state with n particles corresponds to an element $\psi^{(n)}(x_1, \ldots, x_n) \in \mathcal{F}_\mathrm{s}(\mathcal{H})$ with n coordinates in position representation. One can also use a representation in terms of occupation numbers and simply specify a state by all non–vanishing excitation numbers $\{n_{\vec{k}}\}_{\vec{k}}$ of all modes $\vec{k}$. The annihilation and creaction operators annihilate and create a state f respectively according to (Reed and Simon 1975b)

$$(\boldsymbol{b}(f)\psi)^{(n)}(x_1, \ldots, x_n) = \sqrt{n+1} \int_{\mathbb{T}^3} \mathrm{d}x\, \overline{f(x)} \psi^{(n+1)}(x, x_1, \ldots, x_n), \tag{4.37}$$

$$(\boldsymbol{b}^*(f)\psi)^{(n)}(x_1, \ldots, x_n) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} f(x_i) \psi^{(n-1)}(x_1, \ldots, \tilde{x}_i, \ldots, x_n) \tag{4.38}$$

where the tilde in the last line indicates a missing entry. The state that is void of any excitations is the vacuum state $\Omega \in \mathcal{F}_\mathrm{s}(\mathcal{H})$. Any excited state with excitation numbers $(n) := \{n_k\}_{k \in \Sigma}$ with respect to the chosen mode basis results from applying the appropriate number of creation operators

$$\psi^{(n)} = \prod_{k \in \Sigma} \frac{\left(\boldsymbol{b}_k^*\right)^{n_k}}{\sqrt{n_k!}} \Omega. \tag{4.39}$$

This shortly summarizes the standard quantum field theory of a Klein–Gordon real scalar field on Minkowski space. In order to recover the full theory set out at the beginning, we would however need to leave the scale factor a variable.

Starting from the theory on Minkoswki space, the question is how the theory for another value of a is different from the original one with $a = 1$. More precisely, we recognize that the theories for different values of a differ in the frequency $\omega(a)$, and in a global prefactor of the

Hamiltonian. In our notation, the canonical quantum field and its conjugate momentum do not depend on a, but the annihilation and creation operators acquire an a–dependence through the frequency operator $\omega(a)$. As the annihilation operator fixes a particular vacuum state and the associated excited states, these states obviously depend on a. The vacuum state will consequently be denoted by $\Omega(a)$ and the excited states by $\psi^{(n)}(a)$, and they are still related by the analog of equation (4.39) where now $\boldsymbol{b}_k^*(a)$ as well as $\psi^{(n)}(a)$ and $\Omega(a)$ depend on a. To make the relation between the theories more precise, one can compare the annihilation and creation operators for two different values of a. Let therefore $a_1, a_2 \in \mathbb{R}$, and let $f \in L^2(\mathbb{T}^3, \mathrm{d}x)$. Since $\boldsymbol{\Phi}(f)$ and $\boldsymbol{\Pi}_\Phi(f)$ are a–independent, we can use the decomposition of their representations into annihilation and creation operators to deduce that

$$\left[\sqrt{\omega(a_1)}^{-1}\boldsymbol{b}(a_1) + \sqrt{\omega(a_1)}^{-1}\boldsymbol{b}^*(a_1)\right](f) = \left[\sqrt{\omega(a_2)}^{-1}\boldsymbol{b}(a_2) + \sqrt{\omega(a_2)}^{-1}\boldsymbol{b}^*(a_2)\right](f) \tag{4.40}$$

$$\left[\sqrt{\omega(a_1)}\boldsymbol{b}(a_1) - \sqrt{\omega(a_1)}\boldsymbol{b}^*(a_1)\right](f) = \left[\sqrt{\omega(a_2)}\boldsymbol{b}(a_2) - \sqrt{\omega(a_2)}\boldsymbol{b}^*(a_2)\right](f). \tag{4.41}$$

The two equations allow us to represent $\boldsymbol{b}(a_1, f)$ and $\boldsymbol{b}^*(a_1, f)$ in terms of $\boldsymbol{b}(a_2, f)$ and $\boldsymbol{b}^*(a_2, f)$. Therefore, let us define the two differential operators (Schander and Thiemann 2019a)

$$u_\pm(a_1, a_2) := \frac{1}{2}\left[\sqrt{\frac{\omega(a_1)}{\omega(a_2)}} \pm \sqrt{\frac{\omega(a_2)}{\omega(a_1)}}\right], \tag{4.42}$$

which provides us with relations for the annihilation and creation operators given as

$$\boldsymbol{b}(a_1, f) = [u_+(a_1, a_2)\boldsymbol{b}(a_2)](f) + [u_-(a_1, a_2)\boldsymbol{b}^*(a_2)](f), \tag{4.43}$$

$$\boldsymbol{b}(a_1, f) = [u_-(a_1, a_2)\boldsymbol{b}(a_2)](f) + [u_+(a_1, a_2)\boldsymbol{b}^*(a_2)](f). \tag{4.44}$$

For both values of a, one can choose the standard representations on Fock space and define vacuum states $\Omega(a_1)$ and $\Omega(a_2)$ accordingly. The important question is of course how or rather *if* these two vacua and hence the representations of the field theory can be unitarily related.

It turns out that the answer is in the negative, and this will prevent the application of space adiabatic theory to quantum field theoretical models in the first place. We will come back to this problem in chapter 8 when we discuss the first of the quantum field theoretical models of this thesis. In fact, it is possible to perform a perturbative transformation on the whole canonical phase space that allows to relate the two representations in a unitary way. Before, we will give an overview of the backreaction problem in quantum field theory on curved space times, i.e., in the semiclassical regime, to which the two following sections are dedicated.

4.2. Semiclassical Gravity

Semiclassical gravity is a program that builds on the former QFT on CST approach but which is interested in the backreaction excerted from the quantum field fluctuations on the classical gravitational field. The problem was first laid out by Wald (1977), who considered the backreaction from particle creaction on the gravitational field. The first goal in this program is to consistently

define a modified set of Einstein field equations in which the expectation value of the quantum stress–energy tensor $\boldsymbol{T}_{\mu\nu}$ with respect to an appropriate algebraic quantum state ω of the matter fields appears as a source term, i.e., (Ford 2005)

$$\mathcal{R}^{(4)}_{\mu\nu} + \frac{1}{2} g_{\mu\nu} R^{(4)} = 8\pi G \, \omega(:\boldsymbol{T}_{\mu\nu}:), \tag{4.45}$$

where $\mathcal{R}^{(4)}$ and $R^{(4)}$ are the classical four–dimensional Ricci tensor and curvature scalar (cf. chapter 2), G is Newton's constant, and ω a suitable algebraic state as defined in the previous section. The colons indicate the normal ordering of the stress–energy tensor $\boldsymbol{T}_{\mu\nu}$.

Evaluating the right hand side of this equation is of course not a trivial task and is only well defined after a suitable regularization and renormalization procedure. The explicit implementation of such procedures for a suitable set of quantum states ω is the first goal of semiclassical gravity (Ford 2005). The second goal of semiclassical gravity is to solve these equations and to find the improved dynamics of the classical gravitational field that consistently includes the backreaction of the quantum matter fluctuations. The following summary of the basic ideas and results in semiclassical gravity is mainly based on the the textbooks and articles by Ford (2005), Hack (2016), Hu and Verdaguer (2020), and Siemssen (2015). Note also that parts of this summary can be found in (Schander and Thiemann 2021).

Regarding the first of these two goals, difficulties occur due to the divergent structure of the stress–energy tensor $\boldsymbol{T}_{\mu\nu}$ of the quantum fields (Ford 2005): The tensor generically depends on products of operator–valued distributions of the fields at the *same* space time points, for example one is faced with the formal expression $\boldsymbol{\Phi}(x)^2$. In fact, the two–point function $W_2(x,y) := \omega(\boldsymbol{\Phi}(x)\boldsymbol{\Phi}(y))$ is singular at $x = y$ for a generic quantum state ω. In Minkowski space, the solution is to consider the normal ordered operator $:\boldsymbol{\Phi}(x)^2:$ and to realize that the products of the expectation value $\Omega(:\boldsymbol{\Phi}(x)^2:)$ at different points are well–defined for the Minkowski vacuum Ω. More precisely, such expectation values are well–defined distributions such that a smearing with any two test functions is finite. In general curved space times, the Minkowski vacuum is not available but there are different ways of generalizing the procedure and to obtain a meaningful expression for $\omega(:\boldsymbol{T}_{\mu\nu}:)$.

More precisely, in his seminal work Wald (1977) introduced five axioms that are required to hold for a suitable renormalization scheme to give a meaningful expectation value for the stress energy tensor. The first four axioms are automatically satisfied in every locally covariant theory in line with (Brunetti, Fredenhagen, and Verch 2003). However, the fifth one which requires $\omega(:\boldsymbol{T}_{\mu\nu}:)$ to depend on the derivatives of the metric coefficients up to second order (but not higher derivatives) is not generically given (Wald 1978). One explicit regularization scheme is the Hadamard point–splitting method (Brunetti and Fredenhagen 2000; Hollands and Wald 2001) which proceeds in similar lines as the standard Minkowski approach, and which we already alluded to in section 4.1. As before, one considers the normal–orderd version of the stress–energy tensor, and for a Klein–Gordon field, the latter contains products of the operator–valued field distributions. One then separates the space time points at which the fields in $\boldsymbol{T}_{\mu\nu}$ are evaluated and thereby regularizes the theory. The result depends on the distance regulator, conventionally chosen to be the geodesic distance μ between these points. This expression is evaluated in a sufficiently regular state ω before taking the coincidence limit $\mu \to 0$. Physically relevant states

are the Hadamard states, defined such that normal ordered fields have finite expectation values. More precisely, the two–point distributions evaluated on Hadamard states satisfy the microlocal spectrum condition (Brunetti, Fredenhagen, and Kohler 1996; Radzikowski 1996b). As a consequence, their n–point functions are well–defined distributions. Still, these states have a universal divergence (Kay and Wald 1991; Wald 1977), but the idea behind the point–splitting procedure is to identify and subtract these divergencies in a controlled renormalization procedure before taking the coincidence limit. Namely, the divergencies that appear in $\omega(:\boldsymbol{T}_{\mu\nu}:)$ can be absorbed in the gravitational contributions on the left hand side of the semiclassical Einstein equation by a redefinition of the coupling constants such as Newton's constant or the cosmological constant (Ford 2005). Despite the non–unique normal ordering procedure in the first step of the point–splitting regularization, it was shown that this procedure yields a unique result of the renormalized stress–energy tensor up to redefinitions of the coupling constants (Hollands and Wald 2005; Wald 1977, 1978).

For applications in cosmology, the so–called adiabatic regularization procedure (Fulling, Parker, and Hu 1974a,b; Parker and Fulling 1974) is another way to make sense of the formal expression $\omega(:\boldsymbol{T}_{\mu\nu}:)$. This procedure is essentially equivalent to the above Hadamard point–splitting regularization, in particular, they differ only by local curvature tensors (Siemssen 2015). It relies on the use of adiabatic states (Parker 1969) which are only approximately Hadamard but their straightforward construction proves to be useful (Junker and Schrohe 2002). We already pointed out that its underlying idea is to define approximate WKB solutions of the matter field wave equation for a slowly varying cosmological space time up to a certain order in this approximate scheme. It turns out that the expectation value with respect to such an adiabatic vacuum state of fourth order is regularizable, and one can apply a standard regularization and renormalization scheme as before (Fulling, Parker, and Hu 1974a; Hu and Verdaguer 2020).

The result of these regularization procedures are sets of modified Einstein field equations with quadratic curvature terms, e.g., $(R^{(4)})^2$ and $\mathcal{R}^{(4)}_{\mu\nu}(\mathcal{R}^{(4)})^{\mu\nu}$ are added to the original Einstein Lagrangian. For general couplings of the scalar field, these give rise to fourth order derivatives of the metric (Ford 2005) which cannot be completely reabsorbed in the renormalization constants (Hollands and Wald 2001, 2005). Such a theory would require to fix the metric and its first three derivatives on a spacelike hypersurface to have a well–posed initial value problem, and furthermore can lead to instabilites. Such problems can be (partially) avoided by considering only conformally coupled fields both massless or massive. In this case, local and global solutions of the semiclassical Einstein equations exist (Meda, Pinamonti, and Siemssen 2020). We also mention that in general the expectation value of the stress–energy tensor violates the classical, local positive energy conditions of general relativity. It is however possible to satisfy more general non–local energy conditions such as the "averaged null energy condition" (ANEC) (Flanagan and Wald 1996). Care must however be taken when choosing admissible solutions in order to not violate the self–consisteny of the semiclassical equations.

Applications of the semiclassical scheme to cosmological situations are numerous, and we can only discuss a small fraction of them here. In general, these works aim at estimating the backreaction due to matter quantum fields on the cosmological background, mainly restricted to the conformally coupled scalar field case (Siemssen 2015). One kind of effects is related to the non–vanishing trace (hence denoted as trace anomaly) of the stress–energy tensor for quan-

tum fields (Hu and Verdaguer 2020): In fact, for massless conformally coupled fields, the only quantum source in the semiclassical Einstein equations comes from the trace. In this respect, Fischetti, Hartle, and Hu (1979) considered the backreaction effects from a conformally invariant matter field in an FLRW Universe with classical radiation and found that the trace anomaly can soften the cosmological singularity, but not avoid it. Other works in this direction were done by Anderson (1983, 1984, 1985), who also considered the trace effects on the particle horizon. A well–known example of trace anomaly effects from semiclassical gravity is the Starobinsky (1987) cosmological model.

Another application of semiclassical gravity is the study of backreaction of particle creation on the dynamics of the early Universe as already conceived by Wald (1977), see (Hu and Verdaguer 2020): Grishchuk (1977) as well as Hu and Parker (1977) considered the effect of gravitons around the Planck time in an FLRW Universe with a classical isotropic fluid. They use an adiabatic regularization scheme and find that the graviton creation in this model leads to a timely non–local (i.e., history–dependent) backreaction effect given in terms of a non–local damping kernel in the effective Friedmann equation of the classical FLRW cosmology. Similar studies were performed for anisotropic FLRW Universes and it was shown that particle production due to the shear anisotropy will isotropize space time (Hu and Parker 1978; Hu and Verdaguer 2020; Zel'dovich and Starobinsky 1972). Regarding the effects of particle creation in a spatially inhomogeneous but isotropic Universe, we refer to the work by Campos and Verdaguer (1994).

As also discussed in (Schander and Thiemann 2021), we point to more recent works by Finelli, Marozzi, G. P. Vacca, et al. (2002, 2004) who specifically consider a slow–roll (almost de Sitter) phase of the very early Universe and compute a(n) adiabatically renormalized energy momentum tensor of the quantum inflaton, respectively cosmological scalar fluctuations. In case of the cosmological scalar perturbations, they find that the energy momentum tensor is characterized by a negative energy density which grows during inflation and also that backreaction is not a mere gauge artifact.

Further contributions to the topic of semiclassical gravity for cosmological situations were notably made by Dappiaggi, Fredenhagen, and Pinamonti 2008; Dappiaggi, Hack, et al. 2010; Eltzner and Gottschalk 2011; Gottschalk and Siemssen 2018; Hack 2013; Matsui and Watamura 2020; Parker and Raval 1999; Pinamonti 2011, to mention but a few (Schander and Thiemann 2021). Most recently, Meda, Pinamonti, and Siemssen (2020) have made progress on the definition of the semiclassical theory for general couplings by proving existence and uniqueness of solutions in flat cosmological space times with a massive quantum scalar field. We also point to the recent work by Matsui and Watamura (2020) who claim that semiclassical gravity is not appropriate to describe the early Universe. They also provide an extensive list of further references that provide a good account of achievements in the field of semiclassical gravity, again see also (Schander and Thiemann 2021).

Finally, the question remains whether semiclassical gravity is able to capture the relevant physical effects due to quantum backreaction, i.e., in particular whether the expectation value of the energy–momentum tensor can adequately reflect the quantum nature of the matter fields. In fact, just as for the classical backreactions, there is a vicious circle as we specify a certain class of solutions on the gravitational side which we would actually like to determine by the procedure (Hu and Verdaguer 2020). The theory of stochastic (semiclassical) gravity aims at evaluating this

question of validity of the semiclassical approach by including additional "stochastic" quantum contributions from the matter fields.

4.3. Stochastic (Semiclassical) Gravity

The approach of stochastic (semiclassical) gravity is built on the Einstein–Langevin equations which can be seen as an extension of the former semiclassical Einstein equations. In addition to the expectation value of the quantum stress–energy tensor, it includes an effective noise term due to the fluctuations of the quantum matter fields. More precisely, the noise kernel is the expectation value of a tensor that describes the fluctuations of quantum matter fields in curved space times. This section is mainly based on the papers and textbooks by Calzetta, Hu, and Mazzitelli (2001) and Hu and Verdaguer (2008, 2020) to which we also refer for more thorough introductions to the topic. Note again that parts of this summary can also be found in (Schander and Thiemann 2021).

In fact, it was argued that the bare semiclassical approach to gravity could break down when the fluctuations of the stress–energy tensor are large (Ford 1982; Kuo and Ford 1993). Different proposals have been made to quantify this statement (Ford 2000; Hu and Phillips 2000; Hu, Roura, and Verdaguer 2004; Kuo and Ford 1993), and it was asserted that an additional stochastic source should enter the semiclassical Einstein equations to assure the validity of the approach (Hu and Verdaguer 2020). This led to the development of stochastic gravity, inspired by the idea of an open system approach where one divides the system into an environment (here the quantum matter field) and a system (the gravitational classical degrees of freedom) (Hu 1989).

This idea is manifestly reflected in the functional approach to stochastic gravity which creates a link to open system concepts and statistical features such as dissipation, fluctuations, noise and decoherence (Calzetta and Hu 1987; R. Jordan 1986, 1987). It employs a so–called closed time path coarse grained effective action (CTP CGEA) (Hu and Verdaguer 2020) whose basic idea is to compute an influence action that is a functional of the classical metric but which includes the effects of the quantum matter fields by evaluating the matter path integral along a closed time path. By variation with respect to the metric tensor, the influence action yields the expectation value of the quantum stress–energy tensor. The idea is to evaluate this derivation with respect to a linearly perturbed metric field (Hu and Verdaguer 2008) and which gives rise to the equations of motion for the metric perturbations which are sourced by the influence action and hence by the quantum matter effects. They include the contributions from the expectation value of the stress–energy tensor already known from semiclassical gravity as well as an additional noise term.

As already discussed in (Schander and Thiemann 2021), some of the first applications of the CTP CGEA formalism to the backreaction problem in cosmology were performed by Calzetta and Hu (1987, 1989, 1994), (Hu and Verdaguer 2020). Hu and Matacz (1995) derived the Einstein–Langevin equations for the case of a free massive scalar field in a flat FLRW background. The case of a massless conformally coupled field was discussed in (Campos and Verdaguer 1994). The scope of works (see (Hu and Verdaguer 2020)) includes topics such as stochastic inflation where quantum fluctuations present in the noise term backreact on the inflaton field (Calzetta and Hu 1995; Lombardo and Mazzitelli 1996) as well as studies of the reheating phase in inflationary cosmology (Boyanovsky et al. 1995; Ramsey and Hu 1997). The formalism was also used by Sinha

and Hu (1991) to check the validity of the minisuperspace approximation in quantum cosmology.

We also mention that there is yet another way to formulate stochastic gravity (Hu and Verdaguer 2020), namely the so–called axiomatic approach (Martin and Verdaguer 1999) which establishes the link to semiclassical gravity in a more direct way (Martin and Verdaguer 2000). It starts from the renormalized semiclassical Einstein equation discussed in the previous section and introduces an additional Gaussian stochastic tensor field on the right hand side of these equations. This stochastic tensor field is defined through the two–point correlation function of the stress–energy tensor and accounts for the quantum fluctuations of the quantum matter fields. It represents an additional noise term that induces perturbations of the classical metric. The resultant equations of motion for the metric perturbations with the noise as an additional source are the Einstein–Langevin equations.

Like in (Schander and Thiemann 2021), let us also point to one of the most prominent applications of stochastic methods to early Universe cosmology by Starobinsky (1982, 1988). His stochastic inflationary model evaluates backreaction of small scalar field quantum perturbations on the corresponding long wavelength modes (which are assumed to behave classically) by additional stochastic terms in the long wavelength equations of motion. A slow–roll behavior of the background is assumed. Interestingly, it has been shown that the stochastic and the quantum field theoretic approaches to perturbations in the early Universe yield the same results (Finelli, Marozzi, Starobinsky, et al. 2009; Starobinsky and Yokoyama 1994; Tsamis and Woodard 2005). For recent considerations of stochastic inflation beyond the (strict) slow–roll conditions, we refer to the work by Pattison et al. (2019) and references therein.

In both, the semiclassical and the stochastic approaches to backreaction, one aims at incorporating the effects from the quantum matter fields onto the classical curved space times. The first approach is built on the semiclassical Einstein equations, the second one on the Einstein–Langevin equations. Both provide solutions to the backreaction problem for cases with simple (specifically coupled) scalar field matter content but more involved situations are hard to implement due to technical problems and stabilitiy problems. The most important conceptual problem (from our perspective) is of course that the gravitational field is considered being classical while the matter fields are considered as quantum fields. While this represents a seminal progress to incorporate quantum effects of the matter fields in the early Universe, it can and should be questioned whether this somehow incompatible approach (classical and quantum fields treated at the same level) survives the test of future observations, and whether it should be replaced by a more consistent approach – quantum gravity. The topic of backreaction in the light of approaches to quantum gravity is the subject of the next chapter.

5. Quantum Gravity and Cosmology

This chapter reviews methods of quantifying backreaction in non–perturbative approaches to quantum gravity and quantum cosmology in more detail than the introductory chapter. By non–perturbative, we mean that the gravitational field is not split into a fixed, non–dynamical background and (possible) perturbations thereof, e.g., gravitons, but is considered as a dynamical quantity that is consequently subject to a quantization procedure (i.e., we are excluding any approach with a fixed Minkowski background in which only the perturbative gravitons appear as dynamical degrees of freedom). This is of course vital to the concept of backreaction that we have in mind since in such perturbative approaches, there simply cannot occur any backreaction on the background (gravitational) degrees of freedom by definition.

The notion of backreaction is, of course, multifaceted and encompasses various aspects. In this work, we consider backreaction

i) from a homogeneous and isotropic scalar field on an FLRW space time,

ii) from an inhomogeneous scalar field on an FLRW space time, and

iii) from gauge–invariant cosmological perturbations on the homogeneous and isotropic space time and matter scalar field.

In any of these cases, we consider backreactions onto the homogeneous space time degrees of freedom, and possibly on the homogeneous matter degrees of freedom. Since we see the first case rather as an explorative toy model for the two other cases, we can say that our focus is on the quantum backreaction of cosmological perturbations on the homogeneous and isotropic background degrees of freedom. The perturbative scheme that underlies our computations uses the very small ratio of the gravitational (or Newton's) coupling constant G, and an ordinary matter coupling constant λ.

5.1. Planck Mass and Born–Oppenheimer Schemes in Quantum Gravity

Within the usual Born–Oppenheimer scheme on which this work relies, such a perturbative parameter is identified with the ratio of a very small and a very large mass of the system's constituents such as the electron's and the nuclei's mass. One then speaks of a slow heavy subsystem and the fast light subsystem by comparing their average velocities. It is also claimed that the slow system behaves almost classical which is why in various works, the semiclassical limit for the slow subsystem is invoked by e.g., using semiclassical ansatz solutions for the slow sector, see for example (Hagedorn 1980; Teufel 2003). It is however important to distinguish between the adiabatic limit of the Born–Oppenheimer scheme and a semiclassical limit as was pointed out by Teufel (2003). Our work makes this distinction manifest – no semiclassical approximation is used. Other works

on backreaction in quantum gravity employ these schemes simultaneously which of course allows to explore the semiclassical regime but which is less general.

In this section, we focus on the investigations of quantum gravitational and cosmological backreaction that employ a perturbative approach using the reduced Planck mass of gravity $M_{\mathrm{Pl}} \propto G^{-1/2}$ (or rather its inverse) as a pertrubation parameter. The idea that quantum gravity can be considered as a perturbative theory with respect to M_{Pl} has already been introduced by Brout (1987). The first investigations of backreaction in quantum gravity that rely on this expansion were performed in the framework of quantum geometrodynamics (Kiefer 2007; Wheeler 1957), a quantum gravitational field approach based on Einstein's original metric gravity together with an ADM space time split. The idea is to expand the Wheeler–DeWitt equation (a quantum version of Einstein's equations in the $(3+1)$–split) in terms of the ratio of the Planck mass and the matter field mass (Kiefer and T. P. Singh 1991). A different idea, conceptually similar to the schemes considered here, is to use a Born–Oppenheimer type approach relying on the same perturbation parameter. Different considerations of the problem (giving rise to similar results) can be found in the works by Bertoni, Finelli, and Venturi (1996), Brout and Venturi (1989), and Kiefer (1994) (for a summary, see (Kiefer 2007)). The idea of the Born–Oppenheimer approach will be explained in section 6 in great detail, but to understand its use in the given context we present the key ideas. Note that parts of this section resemble the discussion in (Schander and Thiemann 2021).

In quantum geometrodynamics, one starts with the Wheeler–DeWitt equation (i.e., a quantization of the classical constraint equation of gravity) which includes quantum geometry and a quantum matter field (usually a real–valued scalar field). For simplicity, let Q denote the gravitational and q the matter degrees of freedom. The Born–Oppenheimer scheme employs an ansatz solution for the quantum Hamiltonian and momentum constraint of the form (Kiefer 2007)

$$\Psi(q,Q) = \sum_n \chi_n(Q)\psi_n(q,Q) \tag{5.1}$$

where $\{\psi_n(q,Q)\}_n$, $n \in \mathbb{N}$ is supposed to be a known orthonormal basis of the matter Hilbert space that solves the matter part of the constraint and Q is to be considered as an external parameter for this eigenvalue problem. Then one applies the constraints to Ψ and applies some $\psi_k(q,Q)$ from the left (i.e., one considers the inner product of the matter states) (Kiefer 2007). This gives rise to constraint equations for the geometric factors $\chi_n(Q)$ which can be seen as an effective quantum problem for the geometric part, including the backreaction effects of the quantum matter system.

In order to examine a semiclassical limit of the theory (i.e., a matter quantum field theory on curved space times), it is common to employ a WKB ansatz for the geometrical states $\chi_n(Q)$ of the form (Kiefer 2007)

$$\chi_n(Q) = C_n(Q)e^{iM_{\mathrm{Pl}}{}^2 S[Q]}. \tag{5.2}$$

The perturbative scheme in $M_{\mathrm{Pl}}{}^{-1}$ eventually yields the semiclassical Einstein equations. In this sense, these approaches evaluate the backreaction of the quantum matter fields on the quantum or classical geometry.

One can also apply the Born–Oppenheimer and WKB approximations in a different manner. Instead of taking the expectation value with respect to the quantum matter system, one applies the Wheeler–DeWitt constraints on the total Born–Oppenheimer ansatz function and uses the WKB

approximation for the geometrical part. Restricting again to the lowest order with respect to the Planck mass, this yields a quantum constraint for the matter wave function which depends on the classical action (through the WKB ansatz), and derivatives with respect to the spatial metric thereof. The idea of the above–cited works (and also of (Briggs and Rost 2000)) is to introduce an external time parameter that depends on this derivative, hence giving rise to a Schrödinger equation for the matter system that includes the backreaction of the geometry through the geometry–dependent time derivative. In fact, this gives rise to a notion of time in a formerly background independent framework. Such ideas go back to DeWitt (1967) and have been applied to a variety of cosmological situations (see (Kiefer 2007) and references therein). Another approach for recovering a notion of time and a unitary evolution was proposed by Di Gioia et al. (2021) (see also references therein), and it was emphasized that the question has not been given a conclusive answer yet. It is also a different notion of backreaction than the one considered in this thesis.

We emphasize again that these approaches rely on a WKB approximation in order to consider a semiclassical limit. Applications of these works to the inflationary paradigm with perturbations and a discussion of the question of unitary evolution of the perturbations can be found in the work by Chataignier and Krämer (2021) and references therein. In this work, they also consider cosmological perturbations that include gravitational contributions (i.e., the Mukhanov–Sasaki variables). Similar approaches that do not split the system into geometric and matter parts, but include (perturbative) parts of the gravitational degrees of freedom in the fast subsystem and (homogeneous) matter parts in the slow sector were also proposed by Halliwell and Hawking (1987) and A. Vilenkin (1989). This split will also be our choice in chapter 9 of this thesis.

The Born–Oppenheimer approximation was also considered within approaches to quantum gravity that attempt to use connection and flux variables instead of the usual metric variables of Einstein gravity. Giesel, Tambornino, and Thiemann (2009) aimed at an application of the Born–Oppenheimer methods to LQG using holonomy–flux variables or connection–flux variables. As it turns out, this choice of variables prevents the use of the Born–Oppenheimer methods since the flux operators are mutually non–commuting (which is here a prerequisite for the Born–Oppenheimer scheme to work). Instead, they use commuting co–triad variables for the gravity sector and a scalar field for the matter sector. At zeroth order of the scheme, and assuming that the gravitational sector behaves effectively classical, it is possible to derive effective semiclassical Einstein equations that take the backreaction of the quantum matter fields via an expectation value into account. Giesel, Tambornino, and Thiemann (2009) consider their model on a discrete lattice (as it is common practice for approaches to LQG), and thus formally obtain a lattice QFT on a discrete curved space time. They also point to the possibility of pursuing the formal Born–Oppenheimer scheme and computing *quantum* solutions to the gravity sector with the effective backreaction of the quantum matter fields. Finally, they introduce a hybrid approach (similar to the models we consider here) where the gravitational sector is restricted to FLRW solutions and the fast part of the system is given by the matter quantum fields. They also propose to introduce coherent states for the gravitational subsystem in order to make progress in finding solutions. Due to the complexity of the gravity–matter systems, the focus of this work lies on spelling out the conceptual ideas rather than technically carrying out the program in detail.

5.2. Space Adiabatic Methods in Quantum Gravity

More recently, Stottmeister and Thiemann (2016a,b,c) considered similar questions in the context of LQG but employed the more general SAPT scheme (Panati, Spohn, and Teufel 2003). Since in the latter approach, the variables of the slow, gravitational sector are not required to commute (as it was the case in the Born–Oppenheimer approach), it is possible to apply the Born–Oppenheimer ideas also to LQG and related theories. The concrete implementation turns however out to be difficult due to the particular structure of the LQG phase space and represention. More precisely, the phase space of LQG relies on the cotangent bundle T^*G of a compact Lie group G (rather than on a vector space), and the compactness of this group prevents a direct application of the space adiabatic methods. More precisely, it implies that the Weyl quantizations of the local T^*G and the global $G \times \hat{G}$ where $\hat{G}$ is the dual of G need to be distinguished which makes it necessary to choose between local and global structures at various points. Besides, the compactness of the group G prevents an ε–scaling of the position variables, i.e., the transfer of the deformation parameter ε from the momenta to the position variables in the global setting which makes the whole enterprise much more rigid (Stottmeister 2015; Stottmeister and Thiemann 2016b). Solutions to this problem can be derived in the case of abelian groups such as $G = U(1)^n$, $n \in \mathbb{N}$ (Stottmeister and Thiemann 2016b), but for the non–abelian case $G = SU(2)$ of interest in LQG such strategies do not apply. Other open issues of their attempts are related to the underlying graph structure of LQG models and the projective limits of finite dimensional truncations of the gravitational phase space that are needed in order to construct a continuum theory (Stottmeister and Thiemann 2016c). They also point out that a major obstruction to the derivation of a QFT on CST from LQG lies in the inequivalent representations of quantum fields for different gravitational configurations (Stottmeister and Thiemann 2016c). This problem is a generic feature of background dependent quantum field theories as we have seen in the previous chapter. In this work, we present a (perturbative) solution to this problem which makes the application of space adiabatic methods to quantum cosmology possible, and which was already introduced by Castelló Gomar, Martín–Benito, and Mena Marugán (2016), Castelló Gomar, Martín-Benito, and Mena Marugán (2015), and Fernandez–Mendez et al. (2012).

5.3. Born–Oppenheimer in Quantum Cosmology and Decoherence

Now, of course, one can still try to make progress by assuming symmetry reductions, and in fact, the cosmological principle encourages us to do so. We already referred to discussions of the Born–Oppenheimer approach within quantum geometrodynamics, and in particular within its cosmological sector (Chataignier and Krämer 2021; Kamenshchik, Tronconi, and Venturi 2020; Kiefer 2007). In particular, Chataignier and Krämer (2021) consider the quantum gravitational corrections to the power spectra of scalar and tensor perturbations, and succeed in deriving a unitary evolution for the cosmological perturbations by making a particular gauge choice. In this framework, the usual (semiclassical) WKB ansatz is induced in order to recover a time variable. A comparison of different proposals for how to implement the Born–Oppenheimer semiclassical approximation was given by Kamenshchik, Tronconi, and Venturi (2020). We also indicate that Di Gioia et al. (2021) have examined the question of unitary evolution in more detail and

make another proposal for recovering a unitary evolution. Besides, we point to the application of Born–Oppenheimer methods within the spin foam approach to LQC (Rovelli and Vidotto 2008), and point out that Castelló Gomar, Martín–Benito, and Mena Marugán (2016) consider a kind of Born–Oppenheimer approximation in the hybrid approach to LQC which is however conceptually different from ours.

As already pointed out for the quantum gravitational case, many of these approaches rely on a semiclassical (WKB) ansatz solution for the "heavy" homogeneous part of the system, and which is, in fact, not a proper semiclassical state. Besides, it is a specific choice which restricts the theory to a very small range of physical situations. In general, all these approaches rely on a number of different assumptions, e.g., that backreaction is indeed (very) small, see (Castelló Gomar, Martín-Benito, and Mena Marugán 2015) and (Agullo, Ashtekar, and Nelson 2013) for a detailed account of these assumptions in the hybrid and in the dressed metric approaches to LQC respectively. Even if these proposals provide seminal progress in evaluating and incorporating backreaction in quantum cosmology, it is because of these various assumptions, which are in fact hard to control, that we aim at establishing an unambigious scheme that does not build on any of these assumptions.

Before we move on to the presentation of the SAPT scheme in the following chapter, let us also stress that there is an obvious connection between backreaction and decoherence (Schlosshauer 2007). Decoherence (Zeh 1970) is the physical mechanism in which a quantum system looses its quantum mechanical properties (more precisely its coherence, i.e., the definite phase relation between different quantum states) through its interaction with an environmental system. Indeed, in decoherence one aims at finding an effective description of a specific subsystem using the reduced density matrix approach, tracing over the remaining degrees of freedom within the system, and computing its effective dynamics, e.g., by solving associated Lindblad equations (Manzano 2020).

The idea of decoherence can be applied to a quantum gravitational setting in different ways. On the one hand, the environmental system can be composed of *all* inhomogeneous degrees of freedom which in turn induce a quantum–to–classical transition in the purely homogeneous (global) cosmological sector. This concept was first considered by Kiefer (1987) and Paz and Sinha (1991, 1992) and refined by Barvinsky, Kamenshchik, Kiefer, and Mishakov (1999) for the case of cosmological (bosonic) perturbations in an inflationary Universe. Barvinsky, Kamenshchik, and Kiefer (1999) also considered a system with perturbative fermionic degrees of freedom. Similar to the above applications of the Born–Oppenheimer formalism, these approaches rely on a semiclassical WKB approximation, and hence a specific set of ansatz solutions for system's and environmental degrees of freedom. On the other hand, the same reasoning can be applied to the quantum–to–classical transition of the cosmological inhomogeneous modes during inflation (Kiefer, Polarski, and Starobinsky 1998; Polarski and Starobinsky 1996). This decoherence process becomes relevant when the wavelength of the relevant primordial quantum field mode substantially exceeds the Hubble scale H^{-1}. The reasoning of this approach is similar to the previous one and relies on a semiclassical approximation together with the existence of a classical homogeneous background. Besides, both approaches employ a time variable obtained by using the Hamilton–Jacobi equations in the semiclassical WKB approximation.

In fact, it is difficult to compute precise cosmological backreaction effects in perturbative

quantum cosmology without relying on an approximation scheme or a set of specific ansatz solutions, or more generically, to account for *all* relevant interactions in coupled gravity–matter systems. The constraint character of gravity prevents us from using the standard quantum mechanical tools for solving such systems, e.g., there is no a priori given time variable, and besides, the equations are highly non–linear. Even for purely homogeneous and isotropic considerations in quantum cosmology, solutions to the constraint equations are only known for highly simplified systems (independent of the quantization procedure that one chooses). An inclusion of the inhomogeneous quantum fields makes the difficult task of finding (approximate) solutions seemingly impossible, even more the derivation of a semiclassical limit. Finding such a limit, in particular a QFT on CST from full quantum gravity is however indispensable in order to identify the viable candidates for theories of quantum gravity, and to bridge the gap between theory and experiment. As already pointed out in the introduction, the construction of semiclassical, maybe coherent states, for obtaining such a limit is a highly non–trivial endeavor, and has not been successfully accomplished until today. The definition of such a limit for symmetry–reduced cosmological models may be possible, but the approaches considered in this respect mostly neglect the effects of backreaction between the system's constituents.

In the remainder of this thesis, we will advocate the idea of implementing the SAPT approach for making progress regarding these questions. In particular, we will show how this formalism allows us to rigorously implement backreaction into coupled quantum gravity–matter systems, and to hence, also approach the semiclassical limit of quantum gravity in a second step. It is an unambiguous attempt in including such backreaction since it applies, in principle, to different quantum gravitational or cosmological systems, and also the specific quantization underlying the quantum gravity scheme may be modified. SAPT is an inductive scheme which allows to define effective quantum constraints with a considerably simpler structure than the original problem, but whose solutions approximate the true solutions up to an, in principle, indefinitely small error. It includes a formal, natural split between the homogeneous and inhomogeneous quantum degrees of freedom, and which is reminiscent of the split within the semiclassical limit of cosmological QFT on CST. The scheme will hence simplify the remaining steps towards a semiclassical approximation of quantum cosmology. Similar to the Born–Oppenheimer scheme, it uses the inverse Planck mass, or rather the ratio of a matter coupling constant and the Planck mass, as a perturbative parameter.

In the next chapter, we will provide the reader with a detailed review of the Born–Oppenheimer scheme, an introduction to SAPT and all necessary mathematical tools. Besides, we examine the iterative procedure of the scheme, and for reasons of clarity, we apply the scheme to a simple oscillator toy model up to second order in the adiabatic perturbations.

6. Coupled Quantum Systems

Most quantum mechanical systems, in particular those with non–trivial couplings between their internal degrees of freedom, withhold exact analytical or numerical solutions. In certain cases however, consistent approximation schemes provide a mean to extract almost accurate solutions and dynamics. In this chapter, we discuss an approach to approximately solving coupled quantum mechanical systems which have a unifying characteristic: the occurrence of a small, perturbative parameter ε. Here, this parameter will identify the highly differing mass or energy scales of two inherent subsystems. In case of a molecule, it naturally arises as the ratio of the electronic and the nucleonic masses m_e and m_n, $\varepsilon^2 := \frac{m_\mathrm{e}}{m_\mathrm{n}}$. Recall that an electron has a mass of order $m_\mathrm{e} \approx 9.11{\times}10^{-31}$ kg while a nucleon has a mass of order $m_\mathrm{n} \approx 1.67{\times}10^{-27}$ kg, hence, $\varepsilon^2 \approx 5.46{\times}10^{-4} \ll 1$. As we will see in part III of this thesis, also cosmological systems allow for a definition of a perturbative parameter by means of their coupling constants.

This chapter introduces the ideas and techniques of the approximation scheme coined *space adiabatic perturbation theory* (SAPT) (Panati, Spohn, and Teufel 2003) that we are going to extend for the computation of backreaction in quantum cosmology. The chapter and appendix A rely to a large extent on the textbook by Teufel (2003), but also on the works by Dubin, Hennings, and Smith (1980), Chruściński and Jamiołkowksi (2004) and Stottmeister and Thiemann (2016a) among others. Sections 6.6, 6.7 and 6.8 as well as the appendix B are strongly inspired by (Neuser, Schander, and Thiemann 2019; Schander and Thiemann 2019a,c), and partly taken from these references.

The SAPT scheme is a straightforward extension of the Born–Oppenheimer method well–known from molecular physics, and further discussed in section 6.1. Its underlying idea is to exploit the highly differing velocities of nuclei and electrons in a molecule related to the equipartition of kinetic energies in the system: Large masses can statistically be associated with small velocities or more precisely, the averages of the nucleonic and electronic velocities satisfy the relation $\langle v_\mathrm{n} \rangle \approx \varepsilon \langle v_\mathrm{e} \rangle$. It is thus reasonable to speak of the *slow* nucleonic system and the *fast* electronic system, and to use an ansatz of quantum electronic solutions with fixed nucleonic coordinates. It allows to compute an expression for the stationary spectra of the system which however admit errors of order ε.

To analyze the dynamics of the system, it is straightforward to generalize the original Born–Oppenheimer scheme to the first order adiabatic theory (to be discussed below) which permits to give first order error estimates for the dynamical evolution of the system. As the electronic ansatz functions provide suitable approximate solutions which remain almost invariant under the dynamics of the full Hamiltonian, one also speaks of *adiabatic decoupling* of the electron energy bands, and ε is denoted as the adiabatic perturbation parameter. The theory offers however no direct way to improve the first order error estimates, and furthermore, supports only a certain

class of Hamilton operators. It does not cover couplings mediated by non–commuting operators with respect to the slow subsystem.

The idea of the SAPT approach is to introduce a phase space quantization scheme which will lift the above restrictions, see section 6.2 for more details. More precisely, it comes in the form of an operator–valued pseudodifferential calculus to be explained in section 6.3. In sections 6.4 and 6.5, we are ready to introduce and discuss the scheme of SAPT itself which will accompany us throughout the remainder of this thesis, and which represents a successfull extension of the Born–Oppenheimer approximation to *any* perturbative order and for a large range of Hamilton operators and even constraints. Section 6.6 is intended for the iterative execution of the scheme and shows its consistency. In section 6.7, we provide all relevant formulae of SAPT for the type of models examined in the remainder of this thesis and up to second order in the adiabatic perturbations. Finally, we exemplify it with a model of coupled quantum oscillators in section 6.8.

6.1. The Born–Oppenheimer Approximation

6.1.1. Stationary Born–Oppenheimer Theory

The formalism by Born and Oppenheimer (1927) (see also (Born and Huang 1954)) provides a scheme to compute approximate spectra and eigensolutions to coupled quantum systems, most prominently applied to microscopic, molecular systems. The basic idea of the scheme consists in partially projecting the molecular Hamiltonian on a wisely chosen wave function of the electronic subsystem in order to obtain an effective Hamiltonian for the slow nuclei only. A review of this scheme, mostly inspired by Chruściński and Jamiołkowksi (2004, Section 6.3.3.), Panati, Spohn, and Teufel (2007) as well as Stottmeister and Thiemann (2016a, Section II), is the subject of this section.

We choose a simple setting with N nuclei with positions and momenta $(q, P) \in \mathbb{R}^{2N}$ and likewise for the K electrons with positions and momenta $(x, y) \in \mathbb{R}^{2K}$. In the corresponding quantum theory, let us label the quantum operators associated with the nuclei using hats, i.e., by $\hat{q} \in \mathcal{L}(\mathcal{S}_\mathrm{n})$ and $\hat{P} \in \mathcal{L}(\mathcal{S}_\mathrm{n})$ where $\mathcal{S}_\mathrm{n}$ is the space of Schwartz functions in N dimensions and $\mathcal{L}$ denotes the space of linear operators on $\mathcal{S}_\mathrm{n}$. For the electronic subsystem, we define the quantum operators as bold letters, i.e., by $\boldsymbol{x} \in \mathcal{L}(\mathcal{S}_\mathrm{e})$ and $\boldsymbol{y} \in \mathcal{L}(\mathcal{S}_\mathrm{e})$. Thereby, $\mathcal{S}_\mathrm{e}$ is the Schwartz space in K dimensions. $\mathcal{S}_\mathrm{n}$ and $\mathcal{S}_\mathrm{e}$ are subspaces of the so–called nucleonic and electronic Hilbert spaces $\mathcal{H}_\mathrm{s} := L^2(\mathbb{R}^N)$ and $\mathcal{H}_\mathrm{f} := L^2(\mathbb{R}^K)$ on which the respective canonical operators are essentially self–adjoint. The total Hilbert space arises as the tensor product of Hilbert spaces $\mathcal{H} = \mathcal{H}_\mathrm{s} \otimes \mathcal{H}_\mathrm{f}$. The operators on the total Hilbert space $\mathcal{H}$ result from tensor multiplying bounded operators. For example, the Weyl elements associated with the canonical variables become bounded operators on $\mathcal{H}$ by tensor multiplying with a unity operator, i.e., $\exp(i\xi\hat{q}) \to \exp(i\xi\hat{q}) \otimes \mathbf{1}_\mathrm{f}$ or $\exp(i\lambda\boldsymbol{x}) \to \hat{1}_\mathrm{s} \otimes \exp(i\lambda\boldsymbol{x})$ for some $\xi, \lambda \in \mathbb{R}$. Whenever it is clear from the context, we omit such trivial factors. Note that the different presentations of quantum operators for the slow and the fast subsystem (i.e., using hats versus bold letters) is just a convenient tool to distinguish the two subsystems in an obvious way. One could use the same representation on the Hilbert space $L^2(\mathbb{R}^{N+K})$ in fact, this is equivalent (Reed and Simon 1975a):

Remark. Tensor Products of Hilbert Spaces
The unique isomorphism, $L^2(\mathbb{R}^N)\otimes L^2(\mathbb{R}^K) \cong L^2(\mathbb{R}^{N+K})$ gives rise to the unitary mapping $f\otimes g \mapsto g(q)f(x) \in L^2(\mathbb{R}^{N+K})$ for any $f \in L^2(\mathbb{R}^N), g \in L^2(\mathbb{R}^K)$ (Reed and Simon 1975a, p. 50). Besides, for any separable Hilbert space $\mathcal{H}_\mathrm{f}$, there is a unique isomorphism from $L^2(\mathbb{R}^N) \otimes \mathcal{H}_\mathrm{f}$ to $L^2(\mathbb{R}^N, \mathcal{H}_\mathrm{f})$ given by the unitary mapping $f \otimes \varphi \mapsto f(q)\varphi$ for any $f \in L^2(\mathbb{R}^N)$ and $\varphi \in \mathcal{H}_\mathrm{f}$ (Reed and Simon 1975a, Theorem II.10). This motivates to consider a fibre bundle formalism for the joint Hilbert spaces as it views states in the total Hilbert space as functions over $\mathbb{R}^N$ with values in $\mathcal{H}_\mathrm{f}$. A state has the form of a vector field over $\mathbb{R}^N$. The simplest possible field has only *one* non–vanishing value at some point $q_0 \in \mathbb{R}^N$, and can be represented as a delta distribution $\delta_{q_0} \in \mathcal{S}'(\mathbb{R}^N)$ that has a vector $\phi \in \mathcal{H}_\mathrm{f}$ associated to this point. In fact, any vector field or wave function in $L^2(\mathbb{R}^N, \mathcal{H}_\mathrm{f})$ can be represented as a linear combination of the generalized states $\delta_{q_0}\phi(q_0)$ with $q_0 \in \mathbb{R}$ where we allow $\phi \in \mathcal{H}_\mathrm{f}$ to depend on the point of reference q_0 (see (Ballentine 2000; Gel'fand and N. Y. Vilenkin 1964) for the notion of generalized states and rigged Hilbert spaces). In appendix A, we show that this construction yields indeed a complete generalized eigenbasis.

Let us consider a (molecular) Hamilton operator which includes an external magnetic potential, $A : \mathbb{R}^N \to \mathbb{R}$ such that (Teufel 2003)

$$\hat{\boldsymbol{H}} := \frac{\left(\hat{P} + A(\hat{q})\right)^2}{2M} + \frac{(\boldsymbol{y} - A(\boldsymbol{x}))^2}{2m} + V(\hat{q}, \boldsymbol{x}). \tag{6.1}$$

The operator is defined on a dense domain $\mathcal{D}_H \subset L^2(\mathbb{R}^N, \mathcal{H}_\mathrm{f})$. The potential $V(q, x) : \mathbb{R}^{N+K} \to \mathbb{R}$ is in general a complicated function of all configuration variables and mediates the coupling between the nuclei and the electrons (typically, a Coulomb potential). In a first step, the Born–Oppenheimer formalism suggests to split the Hamiltonian into two parts according to

$$\hat{\boldsymbol{H}} := \frac{\left(\hat{P} + A(\hat{q})\right)^2}{2M} + H_\mathrm{f}(\hat{q}, \boldsymbol{x}, \boldsymbol{y}) \tag{6.2}$$

where $H_\mathrm{f}(\hat{q}, \boldsymbol{x}, \boldsymbol{y})$ is the so–called electronic Hamiltonian. Because the potential V in the electronic Hamiltonian solely depends on the commuting position operators $\hat{q}$ with respect to the nucleonic system, it is convenient to make the following considerations. We first assume that for every $q_0 \in \mathbb{R}^N$, there exists a complete eigenbasis $\{\phi_n(q_0)\}_{n\in\mathbb{N}^K}$ of $\mathcal{H}_\mathrm{f}$ such that

$$H_\mathrm{f}(q_0, \boldsymbol{x}, \boldsymbol{y})\, \phi_n(q_0) = E_{\mathrm{f},n}(q_0)\, \phi_n(q_0) \tag{6.3}$$

where the $E_{\mathrm{f},n}(q_0) \in \mathbb{R}$ are the q_0–dependent eigenenergies. For variable q_0, they define the *electronic energy bands*. We assume that the ϕ_n have all multiplicity equal to one. Besides, the energy functions $E_{\mathrm{f},n}(q_0)$ are mutually disjoint functions for every $n \in \mathbb{N}$, i.e., there are no eigenvalue crossings. It is then possible to construct a complete generalized eigenbasis associated with $H_\mathrm{f}(\hat{q}, \boldsymbol{x}, \boldsymbol{y})$ by combining a delta distribution $\delta_{q_0} \in \mathcal{S}'(\mathbb{R}^N)$ with one of the electronic basis states $\phi_\nu(q_0)$, $\nu \in \mathbb{N}$ (Stottmeister and Thiemann 2016a). Cleary, this corresponds to a state in the dual space $\mathcal{S}'(\mathbb{R}^N, \mathcal{H}_\mathrm{f})$ which is only non–vanishing at the point q_0. Formally speaking, one can think of it as having the value $\phi_\nu(q_0)$ there. Since the delta distribution is not in $L^2(\mathbb{R}^N)$, it is necessary to generalize the notion of eigenstates using a rigged Hilbert space, for example $\mathcal{S} \subset \mathcal{H}_\mathrm{s} \subset \mathcal{S}'$. Here, we introduce the distribution $T_{(q_0,\nu)} \in \mathcal{S}'(\mathbb{R}^N, \mathcal{H}_\mathrm{f})$ which acts on states $\Psi \in \mathcal{S}(\mathbb{R}^N, \mathcal{H}_\mathrm{f})$, and

which in a formal integral representation has the form

$$T_{(q_0,\nu)}(\Psi) := \int_{\mathbb{R}^N} \mathrm{d}q\, \delta(q-q_0)\, \langle \phi_\nu(q_0), \cdot \rangle_{\mathcal{H}_\mathrm{f}} \Psi(q) = \langle \phi_\nu(q_0), \Psi(q_0) \rangle_{\mathcal{H}_\mathrm{f}} =: \psi_\nu(q_0). \tag{6.4}$$

It is easy to see that $H_\mathrm{f}(\hat{q}, \boldsymbol{x}, \boldsymbol{y})$ can be lifted to an operator on the larger space $\mathcal{S}'(\mathbb{R}^N, \mathcal{H}_\mathrm{f})$ which yields for every $\Psi \in \mathcal{S}(\mathbb{R}^N, \mathcal{H}_\mathrm{f})$

$$(H_\mathrm{f}(\hat{q}, \boldsymbol{x}, \boldsymbol{y})\, T_{(q_0,\nu)})(\Psi) = \langle H_\mathrm{f}(q_0, \boldsymbol{x}, \boldsymbol{y}) \phi_\nu(q_0), \Psi(q_0) \rangle_{\mathcal{H}_\mathrm{f}} = E_{\mathrm{f},\nu}(q_0) \cdot T_{(q_0,\nu)}(\Psi), \tag{6.5}$$

supporting the idea that the $T_{(q_0,\nu)}$ provide a generalized eigenbasis of the electronic Hamiltonian. The Born–Oppenheimer scheme asks whether these generalized eigenstates remain unchangend under the evolution generated by $\hat{\boldsymbol{H}}$. The answer is in the negative and to see this, let us assume that there exists a solution Ψ^E for $\hat{\boldsymbol{H}}$ with eigenvalue E (Stottmeister and Thiemann 2016a)

$$\hat{\boldsymbol{H}}\, \Psi^E = E\, \Psi^E. \tag{6.6}$$

We project this equation on the distribution $T_{(q_0,\nu)}$ and write it as

$$\begin{aligned} E\, \psi^E_\nu(q_0) &:= T_{(q_0,\nu)}(E\, \Psi^E) = T_{(q_0,\nu)}(\hat{\boldsymbol{H}} \Psi^E) \\ &= \int_{\mathbb{R}^N} \mathrm{d}q\, \delta(q-q_0)\, \langle \phi_\nu(q_0), \cdot \rangle_{\mathcal{H}_\mathrm{f}} \left[\frac{\left(\hat{P} + A(\hat{q})\right)^2}{2M} + H_\mathrm{f}(\hat{q}, \boldsymbol{x}, \boldsymbol{y}) \right] \Psi^E(q). \end{aligned} \tag{6.7}$$

The second electronic term has a trivial solution using equation (6.5) – it is a pure multiplication operator – while the first, kinetic term requires more care. We perform these calculations explicitely in appendix A, and give here only the final result using the matrix elements (Stottmeister and Thiemann 2016a)

$$\mathcal{A}_\nu^{\ n'}(q_0) := -i\, \langle \phi_\nu(q_0), (\nabla_{q_0} \phi_{n'})(q_0) \rangle_{\mathcal{H}_\mathrm{f}}, \tag{6.8}$$

$$D_\nu^{\ n'}(q_0) := \delta_\nu^{\ n'} \left(\nabla_{q_0} + iA(q_0) \right) - i\mathcal{A}_\nu^{\ n'}(q_0), \tag{6.9}$$

and note that the functions $\mathcal{A}_\nu^{\ n'}(q)$ are known as Berry phases in the literature. With $\varepsilon^2 := \frac{m_\mathrm{e}}{m_\mathrm{n}}$ from above, we obtain

$$E\, \psi^E_\nu(q_0) = \sum_{n''} \left(-\frac{\varepsilon^2}{m} \sum_{n'} D_\nu^{\ n'}(q_0)\, D_{n'}^{\ n''}(q_0) + E_{\mathrm{f},\nu}(q_0)\, \delta_n^{\ n''} \right) \psi^E_{n''}(q_0). \tag{6.10}$$

While the electronic, potential term only includes the electronic energy band with the chosen electronic quantum number ν, the kinetic term mixes a priori *all* electronic energy bands. An exact solution could consequently require the computation of an infinite number of matrix elements. To obtain approximate solutions, the Born–Oppenheimer scheme, improved by the Berry–Simon connection (Berry 1984; Simon 1983) or the Mead potential (Mead and Truhlar 1979), ignores these mixing terms such that the only contributing, kinetic matrix element is $D_\nu := D_\nu^{\ \nu}$ (Stottmeister and Thiemann 2016a). In addition, one can perform a perturbative expansion of E and $\psi^E_\nu(q_0)$ in ε. Eventually, it yields reasonable results for the *stationary* molecular spectra. The error estimate can however not be improved by simple means unless we compute the possibly

infinite number of matrix elements. Moreover, one would like to compute the *dynamics* of the problem.

6.1.2. Dynamical First Order Adiabatic Theory

In the previous section, the analysis of the Hamilton operator (6.2) was performed by choosing a particular (generalized) basis state $T_{(q_0,\nu)}$ associated with a point $q_0 \in \mathbb{R}^N$ and an electronic energy band $E_{\mathrm{f},\nu}(q_0)$, and by projecting to a(n unknown) solution of $\hat{\boldsymbol{H}}$. To learn about the molecular dynamics it is more convenient to derive appropriate operator equations. Therefore, let us consider the function $\boldsymbol{H}_\mathrm{f}(q,\boldsymbol{x},\boldsymbol{y})$ on $\mathbb{R}^N$ which arises from the electronic operator $\hat{\boldsymbol{H}}_\mathrm{f}(\hat{q},\boldsymbol{x},\boldsymbol{y})$ by simply replacing the operator $\hat{q}$ with the real parameter q. This next section is a summary of the results in (Teufel 2003).

Accordingly, $\boldsymbol{H}_\mathrm{f}(q,\boldsymbol{x},\boldsymbol{y})$ is a function with values in the linear operators on $\mathcal{H}_\mathrm{f}$, and we additionally assume that it is uniformly bounded and smooth with respect to q, taking values in the bounded, self–adjoint operators on some dense domain $\mathcal{D}_\mathrm{e} \subseteq \mathcal{H}_\mathrm{f}$. Due to the self–adjoint values, it is possible to write the electronic Hamiltonian as a direct integral in the form

$$\hat{\boldsymbol{H}}_\mathrm{f} = \int_{\mathbb{R}^N}^{\oplus} \mathrm{d}q\, \boldsymbol{H}_\mathrm{f}(q,\boldsymbol{x},\boldsymbol{y}) \tag{6.11}$$

such that $\hat{\boldsymbol{H}}_\mathrm{f}$ is a self–adjoint operator on $L^2(\mathbb{R}^K)\otimes\mathcal{D}_e$. More precisely, $\hat{\boldsymbol{H}}_\mathrm{f}$ is a *fibred* operator and naturally acts on the Hilbert space

$$L^2(\mathbb{R}^N)\otimes\mathcal{H}_\mathrm{f} = \int_{\mathbb{R}^N}^{\oplus} \mathrm{d}q\, \mathcal{H}_\mathrm{f} \tag{6.12}$$

in the sense that for a generic wave function $\psi(q,x) \in L^2(\mathbb{R}^K)\otimes\mathcal{D}_e$, the operator $\hat{\boldsymbol{H}}_\mathrm{f}$ acts like $(\hat{\boldsymbol{H}}_\mathrm{f}\psi)(q,x) = \boldsymbol{H}_\mathrm{f}(q,x,-i\partial_x)\psi(q,x)$.

As in the previous section, $\boldsymbol{H}_\mathrm{f}(q)$ admits a complete eigenbasis $\{\phi_n(q)\}_n$ in $\mathcal{H}_\mathrm{f}$ for every value of q and the associated energy bands $E_{\mathrm{f},n}(q)$ can be considered as functions in $\mathbb{R}^N$. Following (Teufel 2003), let us now define a q–dependent projection operator $\boldsymbol{P}_\nu(q) \in \mathcal{B}(\mathcal{H}_\mathrm{f})$ on the electronic Hilbert space $\mathcal{H}_\mathrm{f}$ which is associated with the energy band $E_{\mathrm{f},\nu}(q)$ of $H_\mathrm{f}(q,\boldsymbol{x},\boldsymbol{y})$ for one particular and fixed number $\nu \in \mathbb{N}$. More precisely, for every fixed $q \in \mathbb{R}^N$, it projects any electronic wave function $\phi \in \mathcal{H}_\mathrm{f}$ on the eigenstate $\phi_\nu(q) \in \mathcal{H}_\mathrm{f}$. We promote $\boldsymbol{P}_\nu(q)$ to an operator on the total Hilbert space by the direct integral construction, $\hat{\boldsymbol{P}}_\nu := \int^{\oplus} \mathrm{d}q\, \boldsymbol{P}_\nu(q)$ from above. By definition, $\hat{\boldsymbol{P}}_\nu$ commutes with the fibred, electronic Hamiltonian, and hence $\hat{\boldsymbol{P}}_\nu\mathcal{H}$ is an invariant subspace for the dynamics generated by $\hat{\boldsymbol{H}}_\mathrm{f}$, namely

$$\left[e^{-i\hat{\boldsymbol{H}}_\mathrm{f}s}, \hat{\boldsymbol{P}}_\nu\right] = 0 \tag{6.13}$$

where $s \in \mathbb{R}$ is a microscopic time parameter. Now, let us consider the total Hamiltonian including the kinetic energy contributions of the nuclei. We assume that the magnetic vector potential

$A(q)$ is a bounded and smooth function on $\mathbb{R}^N$, which implies that

$$\hat{\boldsymbol{H}}^\varepsilon := \frac{\varepsilon^2}{2}\left(-i\nabla_q + A(q)\right)^2 + \hat{\boldsymbol{H}}_\mathrm{f}, \tag{6.14}$$

is a self–adjoint operator on its domain of definition $\mathcal{D}(\hat{\boldsymbol{H}}^\varepsilon) = H^2(\mathbb{R}^N) \otimes \mathcal{D}_\mathrm{e}$, where H^2 is the Sobolev Hilbert space. Note that this Hamilton operator is unbounded but for our qualitative statements here, this does not play a substantial role. We will be more precise in this respect in the next sections. As can be shown, the operator $\hat{\boldsymbol{P}}_\nu$ fails to be an orthogonal projection with respect to the total Hamiltonian $\hat{\boldsymbol{H}}^\varepsilon$. Due to the ε–dependent kinetic term, we have that

$$\left[\hat{\boldsymbol{H}}, \hat{\boldsymbol{P}}_\nu\right] \sim \varepsilon, \quad \text{and} \quad \left[e^{-i\hat{\boldsymbol{H}}s}, \hat{\boldsymbol{P}}_\nu\right] \sim \varepsilon|s|. \tag{6.15}$$

The second estimate means that the subspace $\hat{\boldsymbol{P}}_\nu\mathcal{H}$ is not invariant under the dynamics generated by $\hat{\boldsymbol{H}}^\varepsilon$ and states Ψ that are initially in $\hat{\boldsymbol{P}}_\nu\mathcal{H}$ will not remain inside. Only for short time intervals $|s|$, the state approximately stays within $\hat{\boldsymbol{P}}_\nu\mathcal{H}$. In most physical situations however, the interesting molecular dynamics happens on finite *macroscopic* time scales $t := \varepsilon s$. Consequently, the estimate in equation (6.15) leads to results with errors of order $\mathcal{O}(1)$. It is possible to improve this result in several ways which is the aim of the time–adiabatic theory. The important assumption, which continues to play a role in the later applications, consists in presuming an *energy band gap*. In particular, the electronic Hamiltonian should have a discrete band structure, for example

$$E_{\mathrm{f},0}(q) < E_{\mathrm{f},1}(q) < E_{\mathrm{f},2}(q) < ..., \tag{6.16}$$

and in particular such that the energy band $E_{\mathrm{f},\nu}(q)$ for the fixed quantum number ν is separated by a band gap from the remainder of the spectrum for every $q \in \mathbb{R}^N$. More technically, we assume that there is a part $\sigma_\nu(q) \subset \sigma(\boldsymbol{H}_\mathrm{f}(q))$ of the total spectrum σ of $\boldsymbol{H}_\mathrm{f}(q)$ such that there are two bounded functions $f_\pm \in C_\mathrm{b}(\mathbb{R}^N, \mathbb{R})$ that define an interval $I(q) = [f_-(q), f_+(q)]$ such that $\sigma_\nu(q) \subset I(q)$ pointwise, and

$$\inf_{q\in\mathbb{R}^N} \mathrm{dist}\left(I(q), \sigma(\boldsymbol{H}_\mathrm{f}(q)) \setminus \sigma_\nu(q)\right) =: g > 0. \tag{6.17}$$

Of course, it is also possible to make local statements if the energy gap is only satisfied on a certain domain $\mathcal{G} \subset \mathbb{R}^N$. We refer to the book by Teufel (2003) and stick to the global gap condition here. Besides, let us introduce the projection operator $\hat{\boldsymbol{\mathcal{E}}} := \hat{\mathbf{1}}_{(-\infty,\mathcal{E}]}(\hat{\boldsymbol{H}}^\varepsilon)$ which is the spectral projection of $\hat{\boldsymbol{H}}^\varepsilon$ on energies smaller than $\mathcal{E} \in \mathbb{R}$. Then, with the assumption of the gap condition, the time–adiabatic theorem states that there exists a positive constant $C < \infty$ such that

$$\left\|\left[e^{-i\hat{\boldsymbol{H}}^\varepsilon \frac{t}{\varepsilon}}, \hat{\boldsymbol{P}}_\nu\right]\hat{\boldsymbol{\mathcal{E}}}\right\|_{\mathcal{B}(\mathcal{H})} \leq C\,\varepsilon\,(1 + |t|), \tag{6.18}$$

and the norm is for bounded operators on $\mathcal{H}$. Hence, $\hat{\boldsymbol{P}}_\nu\mathcal{H}$ is an approximately invariant subspace with respect to the full dynamics on macroscopic time scales, although $t \ll \frac{1}{\varepsilon}$. The projection on total finite energies is necessary to prevent unbounded kinetic energies, in particular for the nuclei. The result in equation (6.18) supports the idea that subspaces associated with electronic energy bands remain, at least approximately, invariant under the dynamics of $\hat{\boldsymbol{H}}^\varepsilon$.

For concrete applications, it is desirable to learn about the *effective* dynamics within these

subspaces. It is thus useful to define the *diagonal* Hamiltonian

$$\hat{\boldsymbol{H}}^{\varepsilon}_{\mathrm{diag}} := \hat{\boldsymbol{P}}_{\nu}\hat{\boldsymbol{H}}^{\varepsilon}\hat{\boldsymbol{P}}_{\nu} + \hat{\boldsymbol{P}}^{\perp}_{\nu}\hat{\boldsymbol{H}}^{\varepsilon}\hat{\boldsymbol{P}}^{\perp}_{\nu}, \tag{6.19}$$

where $\hat{\boldsymbol{P}}^{\perp}_{\nu} := \hat{\mathbf{1}}_{\mathcal{H}} - \hat{\boldsymbol{P}}_{\nu}$ is the orthogonal compliment of the projector $\hat{\boldsymbol{P}}_{\nu}$. It is easy to see that the diagonal Hamiltonian commutes with $\hat{\boldsymbol{P}}_{\nu}$, and thus leaves the subspace $\hat{\boldsymbol{P}}_{\nu}\mathcal{H}$ invariant under its dynamics. Before we use $\hat{\boldsymbol{H}}^{\varepsilon}_{\mathrm{diag}}$ to analyze the dynamics within $\hat{\boldsymbol{P}}_{\nu}\mathcal{H}$, we first assert that $\hat{\boldsymbol{H}}^{\varepsilon}_{\mathrm{diag}}$ gives indeed a good approximation of the dynamics generated by $\hat{\boldsymbol{H}}^{\varepsilon}$. In fact, it follows from the time–adiabatic theorem that there exists a constant $\tilde{C} < \infty$ such that

$$\left\| \left(e^{-i\hat{\boldsymbol{H}}^{\varepsilon}\frac{t}{\varepsilon}} - e^{-i\hat{\boldsymbol{H}}^{\varepsilon}_{\mathrm{diag}}\frac{t}{\varepsilon}} \right) \hat{\boldsymbol{\mathcal{E}}} \right\|_{\mathcal{B}(\mathcal{H})} \leq \tilde{C}\,\varepsilon\,(1+|\mathcal{E}|)\,(1+|t|). \tag{6.20}$$

This allows to examine $\hat{\boldsymbol{H}}^{\varepsilon}_{\mathrm{diag}}$ and its dynamics on states in the decoupled subspace $\hat{\boldsymbol{P}}_{\nu}\mathcal{H}$ in more detail.

There is however a problem if we want to consider the dynamics of $\hat{\boldsymbol{H}}^{\varepsilon}$ on $\hat{\boldsymbol{P}}_{\nu}\mathcal{H}_{\mathrm{f}}$. In fact, this operator does not preserve the subspace (only up to higher orders in ε). But this is a catastrophe for doing spectral analysis as one cannot compute eigenvalues of an operator which maps out of the considered subspace. It is therefore helpful to switch to a simpler reference subspace which we denote by $\mathcal{R} \subset \mathcal{H}$. A natural reference space is $\mathcal{R} = L^2(\mathbb{R}^N)$, i.e., the nucleonic Hilbert space, and we define a unitary operator $\mathcal{U} : \hat{\boldsymbol{P}}_{\nu}\mathcal{H} \to \mathcal{R}$ with

$$\hat{\boldsymbol{\mathcal{U}}} := \int_{\mathbb{R}^N}^{\oplus} \mathrm{d}q\; \boldsymbol{\mathcal{U}}(q) := \int_{\mathbb{R}^N}^{\oplus} \mathrm{d}q\; \langle \phi_{\nu}(q), \cdot \rangle_{\mathcal{H}_{\mathrm{f}}}. \tag{6.21}$$

The unitary $\hat{\boldsymbol{\mathcal{U}}}$ serves to define an *effective Hamilton operator* on the reference subspace $\mathcal{R}$ given by

$$\hat{H}^{\varepsilon}_{\mathrm{eff}} := \hat{\boldsymbol{\mathcal{U}}}\,\hat{\boldsymbol{P}}_{\nu}\hat{\boldsymbol{H}}^{\varepsilon}\hat{\boldsymbol{P}}_{\nu}\,\hat{\boldsymbol{\mathcal{U}}}^{\dagger} = \frac{\varepsilon^2}{2}\left(-i\nabla_q + A(q)\right)^2 + E_{\mathrm{f},\nu}(q) + \mathcal{O}(\varepsilon^2). \tag{6.22}$$

Evidently, the dynamics generated by $\hat{H}^{\varepsilon}_{\mathrm{eff}}$ on $\mathcal{R}$ has a much simpler form than the dynamics of $\hat{\boldsymbol{H}}^{\varepsilon}$, and there is justified hope that exact solutions are available for this problem. This simpler dynamics can be compared with the original dynamics, and indeed one finds that there exists another constant $\check{C}$ such that

$$\left\| \left(e^{-i\hat{\boldsymbol{H}}^{\varepsilon}\frac{t}{\varepsilon}} - \hat{\boldsymbol{\mathcal{U}}}^{\dagger}\, e^{-i\hat{H}^{\varepsilon}_{\mathrm{eff}}\frac{t}{\varepsilon}}\, \hat{\boldsymbol{\mathcal{U}}} \right) \hat{\boldsymbol{P}}_{\nu}\hat{\boldsymbol{\mathcal{E}}} \right\|_{\mathcal{B}(\mathcal{H})} \leq \tilde{C}\,\varepsilon\,(1+|t|). \tag{6.23}$$

While this result is mathematically not deeper than the estimate in equation (6.20), it shows that the dynamics inside of $\hat{\boldsymbol{P}}_{\nu}\mathcal{H}$ can be formulated by means of a much simpler Hamiltonian and consequently a much simpler Schrödinger equation. In particular, the presence of the spectral gap implies that the dynamics of the nuclei is governed by the effective, electronic potential energy $E_{\mathrm{f},\nu}(q)$. A solution $\psi(q,t)$ to the effective, nucleonic Schrödinger equation

$$i\varepsilon\frac{\mathrm{d}\psi}{\mathrm{d}t} = \hat{H}^{\varepsilon}_{\mathrm{eff}}\psi(t), \quad \psi(t_0) =: \psi_0 \in L^2(\mathbb{R}^N) \tag{6.24}$$

multiplied by the eigenstate $\phi_\nu(q,x)$ is

$$\Psi(t,q,x) = \big(\hat{\boldsymbol{U}}^\dagger \psi\big)(t,q,x) = \psi(t,q)\,\phi_\nu(q,x), \tag{6.25}$$

and yields an approximate solution to the full quantum problem, at least up to errors of order ε and for time scales $t \ll \frac{1}{\varepsilon}$. The question is whether one can improve these error estimates and derive results that are valid for longer time scales. The answer is in the positive, but the techniques employed here are not adequate for this undertaking. Besides, the presented theory only applies to systems for which the coupling operator depends on mutually commuting operators with respect to the slow subsystem. Here, these were the position operators of the N nuclei. The commutativity ensures that the operator has the form of a fibred operator using a direct integral construction. This is however not the case for many interesting problems such as the Dirac equation subject to an external electromagnetic field.

6.1.3. Fibred Operators over Phase Space

We consider and review again an example given in (Teufel 2003): The single particle Dirac theory is modeled on the Hilbert space $L^2(\mathbb{R}^2, \mathbb{C}^4)$ and describes an electron–positron particle with mass m and with two spin directions for the positron and the electron part respectively. In momentum representation, the Dirac Hamiltonian reads

$$\hat{\boldsymbol{H}}_{\mathrm{D}} := \boldsymbol{\alpha} \cdot \big(p - A(i\varepsilon\nabla_p)\big) + m\boldsymbol{\beta} + \phi(i\varepsilon\nabla_p) \tag{6.26}$$

where $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are the standard Dirac matrices composed of the Pauli matrices. $A : \mathbb{R}^3 \to \mathbb{R}^3$ and $\phi : \mathbb{R}^3 \to \mathbb{R}$ are a slowly varying external electromagnetical potential. The techniques of the time adiabatic theory fail for this example because $\hat{\boldsymbol{H}}_{\mathrm{D}}$ cannot be cast into a fibred operator over neither the configuration nor the momentum space: $\hat{p}$ and $\hat{q}$ do not commute. However, one can think of the Dirac Hamiltonian as a function or a "fibration" over the slow *phase space* with values in the bounded operators on $\mathbb{C}^4$, namely

$$\boldsymbol{H}_{\mathrm{D}}(q,p) = \boldsymbol{\alpha} \cdot (p - A(q)) + \boldsymbol{\beta} m + \phi(q). \tag{6.27}$$

In fact, the phase space formulation or more precisely, a phase space quantum mechanics for the slow degrees of freedom will provide a solution to the problem of the Dirac Hamiltonian and also allow for a systematic perturbation theory with respect to the adiabatic parameter ε. This is the subject of sections 6.2, 6.3 and 6.4.

6.1.4. Standard Time–Adiabatic Theory

The reader familiar with the (time) adiabatic theorem might wonder why we refer to the *time*–adiabatic theory in the above considerations. In fact, the time adiabatic theory generically concerns quantum systems with an explicitely time–dependent Hamilton operator $\boldsymbol{H}(t)$. In fact, the standard time–adiabatic theory starts with a family of bounded, self–adjoint Hamilton operators $H(t) \in \mathcal{B}_{\mathrm{sa}}(\mathcal{H})$, $t \in \mathbb{R}$, and is interested in the initial value problem of the unitary propagator

$\boldsymbol{U}^\varepsilon(t,t_0) \in \mathcal{B}(\mathcal{H})$ given by (Teufel 2003)

$$i\varepsilon \frac{\mathrm{d}\boldsymbol{U}^\varepsilon(t,t_0)}{\mathrm{d}t} = \boldsymbol{H}(t)\,\boldsymbol{U}^\varepsilon(t,t_0), \quad \boldsymbol{U}^\varepsilon(t_0,t_0) = \mathbf{1}_{\mathcal{H}} \tag{6.28}$$

which is equivalent to the question of the state evolution $\psi(t) = \boldsymbol{U}^\varepsilon(t,t_0)\psi(t_0)$ with $\psi(t_0), \psi(t) \in \mathcal{H}$. Again based on (Teufel 2003), one can make the following statements: Assuming a spectral gap between some relevant subset $E_\nu(t)$ and the total, time–dependent spectrum $\sigma(t)$ of $\boldsymbol{H}(t)$, and the resulting existence of the orthogonal projection operator $\boldsymbol{P}_\nu(t)$, the time–adiabatic theorem states in its simplest form that there exists a constant $C < \infty$ such that

$$\|(\mathbf{1}_{\mathcal{H}} - \boldsymbol{P}_\nu(t))\,\boldsymbol{U}^\varepsilon(t,t_0)\,\boldsymbol{P}_\nu(t_0)\|_{\mathcal{B}(\mathcal{H})} \leq C\,\varepsilon\,(1 + |t - t_0|). \tag{6.29}$$

A slightly more general version of the theorem defines an adapted, so–called adiabatic unitary propagator $\boldsymbol{U}_a^\varepsilon(t,t_0)$ generated by the adiabatic Hamiltonian $\boldsymbol{H}_a(t)$ which precisely intertwines the spectral subspaces $\boldsymbol{P}_\nu(t)$, i.e.,

$$\boldsymbol{P}_\nu(t)\,\boldsymbol{U}_a^\varepsilon(t,t_0) = \boldsymbol{U}_a^\varepsilon(t,t_0)\,\boldsymbol{P}_\nu(t_0). \tag{6.30}$$

In fact, the adiabatic Hamiltonian corresponds to the diagonal Hamiltonian from above, and the analogous adiabatic theorem states that for some $\boldsymbol{H}(t) \in C_{\mathrm{b}}^2(\mathbb{R}, \mathcal{B}_{\mathrm{sa}}(\mathcal{H}))$ satisfying an energy gap condition, there exists a constant $\tilde{C} < \infty$ such that for all $t, t_0 \in \mathbb{R}$ it holds that

$$\|\,\boldsymbol{U}^\varepsilon(t,t_0) - \boldsymbol{U}_a^\varepsilon(t,t_0)\|_{\mathcal{B}(\mathcal{H})} \leq \tilde{C}\,\varepsilon\,(1 - |t - t_0|). \tag{6.31}$$

This statement ties in with the adiabatic theorem from above, and in fact, the space adiabatic theory is a generalization of this time–adiabatic result. To see this, simply think of the time derivative $i\varepsilon\partial_t$ as a perturbation of the family of Hamiltonians $\boldsymbol{H}(t)$. The proof of the space adiabatic theorem is a generalization of the proof of the time–adiabatic result (6.31) to the case where some $\boldsymbol{H}_0(q)$ is a family of self–adjoint operators on $\mathcal{H}_{\mathrm{f}}$ which leads to the total Hamiltonian

$$\hat{\boldsymbol{H}}^\varepsilon = f(-i\varepsilon\nabla_q) + \int_{\mathbb{R}^N}^{\oplus} \mathrm{d}q\,\boldsymbol{H}_0(q) \tag{6.32}$$

where $f : \mathbb{R}^N \to \mathbb{R}$ corresponds to the perturbation $i\varepsilon\partial_t$ of the time adiabatic case. Put differently, the spectral problem of a time–dependent Hamiltonian $\boldsymbol{H}(t)$ can be understood as the kernel problem of a Hamilton constraint $\hat{\boldsymbol{C}} = \hat{p}_t + \hat{\boldsymbol{H}}(\hat{t})$, where $\hat{p}_t$ is the conjugate momentum of the time operator $\hat{t}$.

It is important to note that the time–dependence in physical systems arises in most cases as an idealization of a coupling to another physical system, that cannot be described in simpler terms. The space adiabatic theory is therefore more generic than the idealized time–adiabatic theory.

6.1.5. The Coherent State Born–Oppenheimer Ansatz

The phase space quantization scheme to be discussed in the following is the core of SAPT and lifts the restriction that the coupling must be mediated by mutually commuting operators in the slow sector. Another possibility to circumvent this limitation is to replace the Dirac delta distributions in the generalized eigenstates $T_{(q_0,n)}$ by some appropriate (overcomplete) basis of coherent states $\widetilde{T}_{(Z_0,n)}$ with $Z_0 \in \mathbb{C}^N$, and which are peaked on classical phase space points (Stottmeister and Thiemann 2016a): More precisely, consider the ε–dependent standard coherent states $\zeta_{Z_0}(q) \in L^2(\mathbb{R}^N)$ associated with the annihilation and creation operators $[\hat{a}_\varepsilon, \hat{a}_\varepsilon^\dagger] = \varepsilon$ of $\hat{q}$ and $\hat{p}$. Then, one might assume that the physical problem admits an operator–valued phase space function $\tilde{\boldsymbol{H}}_0(q, p, \boldsymbol{x}, \boldsymbol{y}) \in C_\mathrm{b}(\mathbb{R}^{2N}, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ such that the associated operator on the full Hilbert space $\mathcal{H} = L^2(\mathbb{R}^N) \otimes \mathcal{H}_\mathrm{f}$ arises as (Stottmeister and Thiemann 2016a)

$$\hat{\boldsymbol{H}}_0(\hat{q}, \hat{p}, \boldsymbol{x}, \boldsymbol{y}) = \hat{\boldsymbol{H}}_0(\hat{a}_\varepsilon, \hat{a}_\varepsilon^\dagger, \boldsymbol{x}, \boldsymbol{y}) = \int_{\mathbb{C}^N} \frac{\mathrm{d}^2 Z}{(\varepsilon\pi)^N} \, \tilde{\boldsymbol{H}}_0(Z, \bar{Z}, \boldsymbol{x}, \boldsymbol{y}) \, \zeta_Z \otimes \langle \zeta_Z, \cdot \rangle_{L^2(\mathbb{R}^N)}. \tag{6.33}$$

If it is possible to solve the eigenvalue problem associated with the operator–symbol $\tilde{\boldsymbol{H}}_0(Z, \bar{Z}, \boldsymbol{x}, \boldsymbol{y})$, one obtains a set of eigensolutions $\{\phi_n(Z, \bar{Z})\}$ in $\mathcal{H}_\mathrm{f}$ with $n \in \mathbb{N}^K$. As before, it is reasonable to build the (overcomplete) family of product states $\{\zeta_{Z_0}(Z) \otimes \phi_n(Z_0, \bar{Z}_0)\}_{n,Z_0} \subset L^2(\mathbb{R}^N, \mathcal{H}_\mathrm{f})$. This ansatz consequently allows to consider operators with a dependence on non–commuting, slow operators, but it comes with some ambiguities due to the overcompleteness of the coherent state basis: In concrete applications, the symbol $\tilde{\boldsymbol{H}}_0(Z, \bar{Z}, \boldsymbol{x}, \boldsymbol{y})$ defined by equation (6.33) is not given a priori so we need to compute it in order to perform a semiclassical analysis. The procedure suggested by the Born–Oppenheimer theory would be to compute the expectation value of $\hat{\boldsymbol{H}}_0(\hat{q}, \hat{p}, \boldsymbol{x}, \boldsymbol{y})$ with respect to the coherent state basis $\{\zeta_{Z_0}(Z) \otimes \psi_n(Z_0, \bar{Z}_0)\}_{n,Z_0}$. Due to the overcompleteness of this basis, the matrix elements obtained by this strategy fail however in general to agree with those that can be derived from $\tilde{\boldsymbol{H}}_0(Z, \bar{Z}, \boldsymbol{x}, \boldsymbol{y})$ (Landsman 1998; Stottmeister and Thiemann 2016a). It is thus not trivial how to obtain the concrete form of $\tilde{\boldsymbol{H}}_0(Z, \bar{Z}, \boldsymbol{x}, \boldsymbol{y})$ from the full Hamilton operator $\hat{\boldsymbol{H}}_0(\hat{q}, \hat{p}, \boldsymbol{x}, \boldsymbol{y})$. Moreover, the computation of the expectation values are often very cumbersome and may even not be possible in some cases. As we will see, SAPT is technically much simpler to implement and uses the semiclassical symbols of operators in a direct manner via the Weyl correspondence.

6.1.6. Summary

This section has illustrated that the standard Born–Oppenheimer theory for stationary spectra and its dynamical time–adiabatic extension admit errors of order ε and require the coupling to be mediated by mutually commuting operators of the slow subsystem. It uses the idea that the fast (electronic) eigensolutions depend parametrically on the nuclei positions which gives rise to a fibre bundle point of view in which any base point q admits a fast (electronic) eigenvalue problem with a fibred (electronic) Hamiltonian. This formalism is thus not adapted to problems such as the one–particle Dirac equation with an external electromagnetic field. The example of the Dirac equation however suggests to consider a fibration over the whole phase space, not only over the slow configutation space. SAPT as developed by Panati, Spohn, and Teufel (2003) uses exactly this idea and establishes a systematic perturbation theory with respect to the adiabatic parameter ε.

To technically realize the perturbative scheme, it employs an ε–scaled phase space quantization for the slow degrees of freedom and develops the equations of motion as an (asymptotic) series in ε. Every coefficient of this power series represents an independent, approximate equation of motion which is usually easier to solve. The phase space quantum mechanics finds its origin in Weyl's quantization prescription (although it does not restrict to his rule of symmetric ordering), and makes contact to the standard Hilbert space representation of quantum theory by means of integral operators. This is the topic of the following section.

6.2. Weyl Quantization and Integral Operators

SAPT is a purely quantum mechanical approach which requires, like any quantum theory, a prescription for associating a quantum observable $\hat{A}$ to a given classical observable $A \in C^\infty(\Gamma, \mathbb{R})$, i.e., to a smooth function on the classical phase space Γ. The representation of a quantum observable can arise in different forms, the most common one is certainly its description as a bounded operator on a (dense domain of a) Hilbert space $\mathcal{H} = L^2(\mathcal{C}, \mathrm{d}\mu)$ where $\mathcal{C}$ is a configuration space and $\mathrm{d}\mu$ an appropriate measure. Another (less well–known) representation is the so–called *phase space* or *deformation quantization* (Bayen et al. 1978a,b; Blaszak and Domanski 2012). Its central idea is to assign to each classical observable a function on phase space, denoted as a "symbol" function and to replace the operator product by a non–commuting product on the corresponding quantum algebra $\mathcal{A}_Q$ of phase space functions. The classification of such symbol functions and the investigation of their properties is known as the theory of pseudodifferential operators ("pseudo", because it exceeds the standard classes of differential operators).

Pseudodifferential calculus was initially developed for the purpose of investigating partial differential equations and particularly singular integral operators on purely mathematical grounds (Kohn and Nirenberg 1965; Mikhlin 1948). Bayen et al. (1978a,b), Hörmander (1979, 1985b), and Howe (1980) and many others subsequently developed the connection and application to quantum mechanics. Formally, the computations within phase space quantum theory can be limited to operations of functions on phase space (like multiplication, inversion etc.). The relation to the common representation of operators acting on Hilbert spaces becomes obvious, if the symbol functions are considered to be part of an integral kernel whose integral with the wave function in $\mathcal{H}$ corresponds to the application of the operator. More precisely, let $\hat{A} \in \mathcal{B}(\mathcal{H})$ be a bounded operator on $\mathcal{H}$ and $\psi \in \mathcal{H}$. Then, the aim is to find an appropriate integral kernel $K_A \in \mathcal{S}'(\mathcal{C}^2)$ in the tempered distributions such that $(\hat{A}\psi)(q) = \int_{\mathcal{C}} \mathrm{d}\mu\, K_A(q, \tilde{q})\, \psi(\tilde{q})$ is a well–defined operation and agrees with the known result from the Hilbert space representation of quantum theory. To understand this relation and also to construct and motivate the computational tools, we will illuminate these basic aspects of the so–called Weyl correspondence and of the pseudodifferential theory. As a starting point, we use the spectral theorem and the Weyl quantization prescription.

SAPT uses this prescription for the slow sector in order to establish a perturbation theory with respect to the physical perturbation parameter ε. The fast sector will be represented using the standard operator quantization. As it turns out, the interplay of these two quantization schemes allows for a systematic treatment of highly non–trivial coupled quantum systems. The resulting theory works with *operator–valued* symbol functions, in contrast to the original pseudodifferential

theory of scalar–valued symbols. This requires the extension of the initial results of the scalar–valued symbolic calculus. We start with a review of the original, scalar–valued symbols and the Weyl correspondence. The following introduction and overview of the topic is inspired by and based on the textbooks by Dubin, Hennings, and Smith (1980, Chapter 8) and by Folland (1989, Chapter 2) as well as by the paper by Blaszak and Domanski (2012)

6.2.1. Weyl Quantization

Consider a one–dimensional system whose position and momentum operators $\hat{q}$ and $\hat{p}$ act as operators on appropriately dense domains of the Hilbert space $\mathcal{H} = L^2(\mathbb{R}, \mathrm{d}q)$. It is often more convenient to work with their associated one–parameter unitary groups $U_\eta(\hat{q})$ and $V_\xi(\hat{p})$ where η and ξ are real parameters which arise from the quantization of the functions $U_\eta(q) = e^{i\eta q}$ and $V_\xi(p) = e^{i\xi p}$ with respect to q and p. The spectral theorem for the operators $\hat{q}$ and $\hat{p}$ together with the corresponding spectral calculus provide a representation of these operators by means of the projection–valued spectral measures $\mathrm{d}\hat{\Pi}_{\hat{q}}$ and $\mathrm{d}\hat{\Pi}_{\hat{p}}$, for example $U_\eta(\hat{q}) = \int_{\sigma(\hat{q})} U_\eta(\lambda)\,\mathrm{d}\hat{\Pi}_{\hat{q}}(\lambda)$, and $\sigma(\hat{q}) = \mathbb{R}$ is the spectrum of $\hat{q}$ (Dubin, Hennings, and Smith 1980). This account of the unitary group elements and the spectral calculus for generic functions $f(\hat{q})$ (or equivalently $g(\hat{p})$) suggests to establish an operator–valued Fourier inversion formula to represent an operator function $f(\hat{q})$ for any $f \in \mathcal{S}(\mathbb{R})$ as (Dubin, Hennings, and Smith 1980)

$$f(\hat{q}) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \check{f}(\eta)\, U_\eta(\hat{q})\, \mathrm{d}\eta \tag{6.34}$$

where $\check{(\cdot)}$ denotes the Fourier transform for Schwartz functions. The Fourier transform also extends uniquely to linear automorphisms of $\mathcal{S}'(\mathbb{R})$. This formula directly follows from employing the Fourier transformation formula and the spectral representation of the unitary group element $U_\eta(\hat{q})$ from above. An equivalent formula holds for momentum–valued functions $g(\hat{p})$. Since in quantum mechanics, position and momentum do not commute, the quantization of mixed operators like $\hat{A} := A(\hat{q}, \hat{p})$ with $A(q, p) \in \mathcal{S}(\mathbb{R}^2)$ is ambivalent. The proposed quantization schemes with the one–parameter unitary groups and the Fourier inversion formula only allow to realize purely $\hat{q}$– or $\hat{p}$–ordered quantization schemes, such as the $\hat{q}$–ordered version of $\hat{A}$ (Dubin, Hennings, and Smith 1980)

$$\hat{A} = \frac{1}{2\pi} \iint_{\mathbb{R}^2} \mathrm{d}\eta\, \mathrm{d}\xi\, \check{A}(\eta, \xi)\, U_\eta(\hat{q}) V_\xi(\hat{p}) \tag{6.35}$$

where $\check{A}$ is the Fourier transform with respect to both q– and p–variables. In fact, this represents the generalization of the standard polynomial $\hat{q}$– and $\hat{p}$–ordered quantization schemes.

To obtain a more symmetric operator ordering and to map real–valued phase space functions onto self–adjoint operators, Weyl (1927) proposed a different ordering prescription by considering the unitary group elements $U_\eta(\hat{q})$ and $V_\xi(\hat{p})$ as being the elements of special subgroups of the more generic Weyl group with elements $W_{(\eta,\xi)}(\hat{q}, \hat{p}) = e^{i(\eta\hat{q} + \xi\hat{p})}$. In particular, $U_\eta = W_{(\eta,0)}$ and $V_\xi = W_{(0,\xi)}$. The quantization prescription for a function $A(q, p)$ is given by (Dubin, Hennings, and Smith 1980)

$$A(q, p) \mapsto \hat{A} = \frac{1}{2\pi} \iint_{\mathbb{R}^2} \mathrm{d}\eta\, \mathrm{d}\xi\, \check{A}(\eta, \xi)\, e^{i(\eta\hat{q} + \xi\hat{p})}, \tag{6.36}$$

and we note that this is a unitary isomorphism from $L^2(\mathbb{R}^2)$ to the space of Hilbert–Schmidt operators on $L^2(\mathbb{R})$. For concrete applications to wave functions $\psi(q)$ in (a dense domain of) the Hilbert space $L^2(\mathbb{R})$, we employ the standard representation of position and momentum operators as multiplication $(\hat{q}\psi)(q) = q \cdot \psi(q)$, and as derivation $(\hat{p}\psi)(q) = -i\hbar(\partial_q\psi)(q)$ operators. Accordingly, the Weyl element $W_{(\eta,\xi)}(\hat{q},\hat{p})$ evaluates to $\left(e^{i(\eta\hat{q}+\xi\hat{p})}\psi\right)(q) = e^{i\hbar(\eta\xi)/2}e^{i\eta q}\,\psi(q+\hbar\xi)$ for any smooth $\psi \in L^2(\mathbb{R})$. This suggests to represent the operator $\hat{A}$ as an integral operator with a corresponding integral kernel K_A. To see this, let us restrict $\psi(q) \in \mathcal{S}(\mathbb{R})$ to be Schwartz, and let $A(q,p) \in \mathcal{S}'(\Gamma)$ be a tempered distribution. Then, the Schwartz kernel theorem states that there is indeed a unique linear operator, $\hat{A} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}'(\mathbb{R}) : \psi \mapsto (\hat{A}\psi)$ with (Teufel 2003)

$$(\hat{A}\psi)(q) = \int_{\mathbb{R}} \mathrm{d}\tilde{q}\, K_A(q,\tilde{q})\,\psi(\tilde{q}) = \frac{1}{2\pi\hbar}\iint_{\mathbb{R}^2} \mathrm{d}\tilde{q}\,\mathrm{d}\xi\, A\Big(\frac{1}{2}(q+\tilde{q}),\xi\Big)e^{i\xi(q-\tilde{q})/\hbar}\psi(\tilde{q}), \tag{6.37}$$

where the kernel $K_A(q,\tilde{q}) \in \mathcal{S}'(\mathbb{R}^2)$ is a tempered distribution. The related assignment, $\hat{W} : \mathcal{S}(\mathbb{R}^2) \to \mathcal{B}(L^2(\mathbb{R}))$ which maps a Schwartz function $A(q,p) \in \mathcal{S}(\mathbb{R}^2)$ on phase space to the corresponding operator $\hat{A} \in \mathcal{B}(L^2(\mathbb{R}))$ on $L^2(\mathbb{R})$ via relation (6.37) is known as the *Weyl correspondence*. Consequently, the knowledge of the function A suffices to uniquely determine the corresponding Weyl quantization $\hat{A}$ without computing the explicit representation on the Hilbert space $L^2(\mathbb{R})$.

6.2.2. Phase Space Quantum Mechanics

To define a quantum theory exlusively as a theory of phase space functions, one also needs to transfer the algebraic structures of the quantum theory to phase space. Our following discussion is mostly a summary of (Blaszak and Domanski 2012), and more details can be found in that reference.

In the classical theory, the Poisson manifold $(\Gamma,\mathcal{P})$ consisting of a smooth phase space manifold Γ, together with the algebra $C^\infty(\Gamma)$ of smooth functions on Γ and the Poisson structure $\mathcal{P}$ define the dynamics of the underlying classical system. Here, the Poisson structure is simply the bilinear Poisson Lie bracket $\{\cdot,\cdot\} : C^\infty(\mathbb{R}^2) \times C^\infty(\mathbb{R}^2) \to C^\infty(\mathbb{R}^2)$. Starting from this classical phase space algebra $\mathcal{A}_\mathrm{c} := (C^\infty(\mathbb{R}^2),\{\cdot,\cdot\},\cdot)$ where "$\cdot$" denotes the commutative pointwise product of phase space functions, the quantum theory replaces the pointwise product by an appropriate, non–commutative "star" product which we denote by "$\star_\hbar$". Since the star product should correspond to the pullback of the operator product to phase space, it is uniquely defined as soon as the operator ordering is fixed. Accordingly, the Poisson bracket transforms into the pullback $[\cdot,\cdot]_\hbar$ of the quantum commutator of operators.

Hence, we define a *quantum* phase space algebra $\mathcal{A}_\mathrm{Q} := (C^\infty(\mathbb{R}^2),[\cdot,\cdot]_\hbar,\star_\hbar)$ for which the star product is a non–commutative and associative relation on $C^\infty(\mathbb{R}^2)$, and the quantum Poisson bracket satisfies the relation $-i\hbar\,[f_1,f_2]_\hbar = (f_1 \star_\hbar f_2 - f_2 \star_\hbar f_1)$ for all $f_1, f_2 \in C^\infty(\mathbb{R}^2)$ which is a natural requirement in order to make contact with standard quantum mechanics (Blaszak and Domanski 2012). One can interpret this procedure as a *deformation quantization* since the star product and the quantum Poisson bracket arise as deformations of the pointwise product and the classical Poisson bracket in the limit $\hbar \to 0$. In particular, the scheme assumes for all f, f_1, $f_2 \in C^\infty(\mathbb{R}^2)$ that (Blaszak and Domanski 2012)

i) $f_1 \star_\hbar f_2 = f_1 \cdot f_2 + o(\hbar)$,

ii) $[f_1, f_2]_\hbar = \{f_1, f_2\} + o(\hbar)$,

iii) $f \star_\hbar 1 = 1 \star_\hbar f = f$.

Given these conditions, the concrete form of the star product defines a quantum theory with a choice of operator ordering. One particularly simple and intuitive class of star products are the *Moyal* products. A Moyal proudct carries the form of a power series expansion in $\hbar$, i.e., $f_1 \star_\hbar f_2 := \sum_{j\in\mathbb{N}} \hbar^j B_j(f_1, f_2)$ where $B_j : \mathcal{A}_\mathrm{Q} \times \mathcal{A}_\mathrm{Q} \to \mathcal{A}_\mathrm{Q}$ are bilinear operators satisfying $B_0(f_1, f_2) = f_1 f_2$, and $B_1(f_1, f_2) - B_1(f_2, f_1) = \{f_1, f_2\}$. The higher order contributions depend on the concrete choice of operator ordering in the quantum theory. One particular subclass of Moyal products has the form of an exponential (Blaszak and Domanski 2012)

$$(f_1 \star_\hbar f_2)(q,p) = \exp\left(i\hbar\sigma\,\partial_q\partial_\xi - i\hbar\bar\sigma\,\partial_p\partial_x\right) f_1(q,p)\, f_2(x,\xi)\Big|_{x=q,\xi=p} \tag{6.38}$$

where the parameters $\sigma \in \mathbb{R}$, and $\bar\sigma = 1 - \sigma \in \mathbb{R}$, parametrize different orderings. This class includes the common Weyl ordering with $\sigma = \frac{1}{2} = \bar\sigma$.

The crucial idea of SAPT is to exploit this $\hbar$–expansion and to supplement it by an additional factor ε which may arise, like for the molecular systems, as the ratio of two inherent masses. In general, let us associate a set of canonical variables (q, P) on the "slow" phase space Γ_s with a heavy mass $M > 0$, and let (x, y) be the canonical pair in the "fast" phase space Γ_f associated with a mass $0 < m \ll M$ such that $\varepsilon^2 := \frac{m}{M} \ll 1$. Using the equipartition theorem, the theory admits that on (statistical) average $\langle y^2\rangle \approx \varepsilon^2\langle P^2\rangle$. It seems thus intuitive to define a *rescaled* momentum $p := \varepsilon P$ such that $\langle p^2\rangle \approx \langle y^2\rangle$.

This redefinition of variables generates a rescaling of the canonical Poisson bracket $\{q, p\} = \varepsilon$, and similarly for the quantum commutator of the associated quantum theory. In particular, we have the rescaled commutation relation $[\hat q, \hat p]_\mathrm{s} = -i\hbar\varepsilon\,\hat 1_\mathrm{s}$ for the position operator $\hat q \in \mathcal{L}(\mathcal{S})$ and respectively for the rescaled momentum operator $\hat p \in \mathcal{L}(\mathcal{S})$, where $\mathcal{S}$ is the one–dimensional Schwartz space. In a deformation quantization scheme of the slow subsystem, the rescaling of the momentum operator is tantamount to a rescaling of Planck's constant $\hbar \to \varepsilon\hbar$ as can easily be deduced from the rescaled definition of the commutator relation above. This has important consequences for the whole phase space quantization scheme, because the power series expansions for the star product and the quantum Poisson bracket can now be considered as to be with respect to the parameter $\tilde\varepsilon := \varepsilon\hbar$. This allows to couple the two subsystems order by order in an ε–expansion in the "adiabatic" limit $\varepsilon \to 0$.

To simplify the analysis, the scheme sticks to the standard Hilbert space representation for operators with respect to the fast subsystem while it employs the phase space representation for the slow subsystem. Quantum operators of the fast subsystem will be indicated by bold letters, e.g., $\boldsymbol{x} \in \mathcal{L}(\mathcal{S})$ and $\boldsymbol{y} \in \mathcal{L}(\mathcal{S})$. Although the scheme employs the phase space scheme for the slow subsystem, recall that a standard analysis of the theory on the total Hilbert space $\mathcal{H} := \mathcal{H}_\mathrm{f} \otimes \mathcal{H}_\mathrm{s}$ is possible by means of the above–introduced Weyl correspondence. Instead of defining quantum operators for the coupled theory as (a sum of) tensor products $\hat A \otimes \boldsymbol{B} \in \mathcal{B}(\mathcal{H})$ of bounded operators $\hat A \in \mathcal{B}(\mathcal{H}_\mathrm{s})$ and $\boldsymbol{B} \in \mathcal{B}(\mathcal{H}_\mathrm{f})$ on the respectively slow and fast Hilbert spaces $\mathcal{H}_\mathrm{s}$ and $\mathcal{H}_\mathrm{f}$, the partial phase space scheme intertwines the representation with quantum phase space

functions and operators on Hilbert spaces. More precisely, quantum observables will have the form of *operator–valued functions on the slow phase space*, i.e., they belong to $C^\infty(\Gamma_\mathrm{s}, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ and take the form $\boldsymbol{A}(q,p) \in C^\infty(\Gamma_\mathrm{s}, \mathcal{B}(\mathcal{H}_\mathrm{f})) = C^\infty(\mathbb{R}^2, L^2(\mathbb{R}))$ (Teufel 2003). The analysis of such operators is the subject of the operator–valued pseudodifferential calculus.

6.3. Operator–Valued Pseudodifferential Calculus

Pseudodifferential calculus for operator–valued symbols as introduced by Panati, Spohn, and Teufel (2003) and detailed by Teufel (2003, Appendix A) is in many respects directly related to the original scalar–valued calculus. The following section is a summary of the relevant notions and definitions provided in (Teufel 2003, Appendix A) to which we refer for more details.

Let $\mathcal{H}$, $\mathcal{H}_1$ and $\mathcal{H}_2$ be separable Hilbert spaces and $\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ the space of bounded linear operators from $\mathcal{H}_1$ to $\mathcal{H}_2$. Let $\boldsymbol{A}$ be a $\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$–valued Schwartz function on $\mathbb{R}^2$, in particular $\boldsymbol{A} \in \mathcal{S}(\mathbb{R}^2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$. Analogous to the scalar–valued case, the function $\boldsymbol{A}(q,p)$ gives rise to an operator $\hat{\boldsymbol{A}} : L^2(\mathbb{R}, \mathcal{H}_1) \to L^2(\mathbb{R}, \mathcal{H}_2)$ by means of the Weyl correspondence. For a wave function $\psi \in \mathcal{S}(\mathbb{R}, \mathcal{H}_1)$, this operator is given by

$$(\hat{\boldsymbol{A}}\psi)(q) = \frac{1}{2\pi\varepsilon} \int_{\mathbb{R}^2} \mathrm{d}\xi \, \mathrm{d}\tilde{q} \, \boldsymbol{A}\left(\frac{1}{2}(q+\tilde{q}), \xi\right) e^{i\xi(q-\tilde{q})/\varepsilon} \, \psi(\tilde{q}). \tag{6.39}$$

It is possible to extend the space of symbol functions for which the Weyl quantization (6.39) yields a well–defined operator on the space of Schwartz functions $\psi \in \mathcal{S}(\mathbb{R}, \mathcal{H}_1)$. We introduce the special symbols by Hörmander in definition 6.1, as well as the more general symbols in definition 6.3 which encompass Hörmander's symbols.

Definition 6.1. Hörmander's Symbols
A function $\boldsymbol{A} \in C^\infty(\mathbb{R}^2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ belongs to Hörmander's symbol class $S^m_\rho(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ with $m \in \mathbb{R}$ and $0 \leq \rho \leq 1$, if for every $\alpha, \beta \in \mathbb{N}$, there exists a positive constant $C_{\alpha,\beta}$ such that

$$\sup_{q\in\mathbb{R}} \left\| (\partial_q^\alpha \partial_p^\beta \boldsymbol{A})(q,p) \right\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)} \leq C_{\alpha,\beta} \langle p \rangle^{m-\rho|\beta|}, \quad \forall p \in \mathbb{R} \tag{6.40}$$

where $\langle p \rangle := (1+p^2)^{1/2}$.

Note that these symbols need to be bounded functions with respect to the configuration variable q, while their at most polynomial growth with respect to the momentum decreases with every derivative with respect to p. This definition, and many other similar definitions of symbol classes, find their motivation in the pseudodifferential calculus for differential operators with non–constant coefficients. Therefore, let $P(x,D)$ be a differential operator with non–constant coefficients and D the differential operator associated with the configuration variable x (Hörmander 1985b): To find solutions $u(x)$ to the differential equation $(P(x,D)u)(x) = f(x)$, it is reasonable to use the ansatz $u = Af$, with $A = A(x,D)$ being a pseudodifferential operator itself. As it turns out, the symbol function $a(x,\xi)$ associated with this operator provides a reasonable approximation and appropriate error estimates for the solution whenever it is of the above symbol type. This is because one seeks approximations whose errors decay asymptotically for large $|p|$ like $|p|^{-k}$

for some $k \in \mathbb{N}$, and the Hörmander symbol functions guarantee just that. For applications in physics, for example in quantum mechanics, there are other limits than the ($|p| \to \infty$)–limit which are of interest for the concrete problem, e.g., the so–called semiclassical limit $\hbar \to 0$, or the adiabatic limit $\varepsilon \to 0$ considered here. Consequently, asymptotic expansions are with respect to these physical parameters and physical problems allow for more generic bounds than the $\langle p \rangle^m$–functions. To have classes of symbols that allow to define a topology and well–defined compositions of symbols, it is reasonable to define them by means of a more generic class of "order" functions.

Definition 6.2. Order Functions
A function $\omega : \mathbb{R}^2 \to [0, +\infty)$ is called an order function if there are constants $C_0 > 0$ and $N_0 > 0$ such that

$$\omega(x) \leq C_0 \langle x - y \rangle^{N_0} \omega(y), \quad \forall x, y \in \mathbb{R}^2. \tag{6.41}$$

The definition consequently gives rise to more generic symbol classes, namely

Definition 6.3. Generic Symbol Classes
A function $\boldsymbol{A} \in C^\infty(\mathbb{R}^2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ belongs to the generic symbol class with order function ω, if for every $\alpha, \beta \in \mathbb{N}$ there exists a positive constant $C_{\alpha,\beta}$ such that

$$\left\| (\partial_q^\alpha \partial_p^\beta \boldsymbol{A})(q,p) \right\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)} \leq C_{\alpha,\beta}\, \omega(q,p), \quad \forall q, p \in \mathbb{R}. \tag{6.42}$$

Note that Hörmander's symbol classes fall in the generic class with $\omega(p) = \langle p \rangle^m$. The advantage of introducing symbol classes is that they are Fréchet spaces with a topology provided by a family of seminorms. These seminorms are given by the minimal constants $C_{\alpha,\beta} > 0$ in equations (6.40) and (6.42). For example, the seminorms in the special case of Hörmander's symbols are

$$\|\boldsymbol{A}\|_k^{(m)} = \sup_{|\alpha|+|\beta| \leq k} \sup_{q,p \in \mathbb{R}} \langle p \rangle^{-m+\rho|\beta|} \left\| (\partial_q^\alpha \partial_p^\beta \boldsymbol{A})(q,p) \right\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)}, \quad k \in \mathbb{N}. \tag{6.43}$$

As in the case of scalar–valued symbol functions, the Weyl quantization of any symbol $\boldsymbol{A} \in S^m_\rho(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ or $\boldsymbol{A} \in S^\omega(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ defines a continuous operator $\hat{\boldsymbol{A}}$ from $\mathcal{S}(\mathbb{R}, \mathcal{H}_1)$ to $\mathcal{S}(\mathbb{R}, \mathcal{H}_2)$ (Teufel 2003, p. 207). Moreover, this mapping extends to a continuous mapping from $\mathcal{S}'(\mathbb{R}, \mathcal{H}_1)$ to $\mathcal{S}'(\mathbb{R}, \mathcal{H}_2)$. These Weyl quantizations form the class of operators

$$\mathrm{OPS}^\omega := \left\{ \hat{W}_\varepsilon(\boldsymbol{A}) : \boldsymbol{A} \in S^\omega(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)) \right\} \tag{6.44}$$

or OPS^m_ρ for the more specific Hörmander symbols. A useful property of these operators is that they are bounded as operators on $L^2(\mathbb{R}, \mathcal{H}_1)$ whenever the corresponding symbol function is a bounded function on phase space. This is the content of the following proposition.

Proposition 6.1. Calderon–Vaillancourt
For every *bounded* operator–valued function $\boldsymbol{A} \in C^3_{\mathrm{b}}(\mathbb{R}^2, \mathcal{B}(\mathcal{H}))$, there exists a constant $C_{\mathrm{d}} < \infty$ such that

$$\left\| \hat{\boldsymbol{A}} \right\|_{\mathcal{B}(L^2(\mathbb{R},\mathcal{H}))} \leq C_{\mathrm{d}} \|\boldsymbol{A}\|_{C^3_{\mathrm{b}}}. \tag{6.45}$$

As a consequence of this theorem, the Weyl quantization of symbol functions in $S^0(\mathcal{B}(\mathcal{H}))$ considered as the map $\hat{W}_\varepsilon : S^0(\mathcal{B}(\mathcal{H})) \to \mathcal{B}(L^2(\mathbb{R}, \mathcal{H}))$ is continuous with respect to the Fréchet

topology of seminorms on $S^0(\mathcal{B}(\mathcal{H}))$. Besides, it is possible to make a statement about the (essential) self–adjointness of symbol operators.

Proposition 6.2. Essential Self–Adjointness
Let $\boldsymbol{A} \in S^{\omega}(\mathcal{B}(\mathcal{H}))$ such that $\boldsymbol{A} + i\,\mathbf{1}_{\mathrm{s}}$ is elliptic in the sense that $\|\boldsymbol{A}(q,p) + i\,\mathbf{1}_{\mathrm{s}}\| \geq C\,\omega(q,p)$ for some $C > 0$. Then, $\hat{\boldsymbol{A}}$ is essentially self–adjoint on $\mathcal{S}(\mathbb{R},\mathcal{H})$ for ε sufficiently small. In particular, for $\boldsymbol{A} \in S^0_0(\mathbb{R},\mathcal{B}_{\mathrm{sa}}(\mathcal{H}))$, i.e., $\boldsymbol{A}$ is a bounded function on phase space with values in the self–adjoint operators on $\mathcal{H}$, then $\hat{A} \in \mathcal{B}_{\mathrm{sa}}(L^2(\mathbb{R},\mathcal{H}))$ is bounded and self–adjoint.

Note that the latter statement holds for any symbol $\boldsymbol{A} \in S^0_\rho(\mathbb{R},\mathcal{B}_{\mathrm{sa}}(\mathcal{H}))$ because $S^m_\rho \subseteq S^m_{\rho'}$ for any $\rho \geq \rho'$. Further important statements of the pseudodifferential calculus concern the composition of symbol functions and their Weyl quantizations. As we have outlined before, the symbol classes admit well–defined products on phase space. The pointwise product $\boldsymbol{A}\cdot\boldsymbol{B}$ of the two symbols $\boldsymbol{A} \in S^{m_1}_\rho(\mathcal{B}(\mathcal{H}_2,\mathcal{H}_3))$ and $\boldsymbol{B} \in S^{m_2}_\rho(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2))$ is in the symbol class $S^{m_1+m_2}_\rho(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_3))$ for every $m_1,\, m_2 \in \mathbb{R}$. Similarly, the pointwise product of symbols $\boldsymbol{A} \in S^{\omega_1}(\mathcal{B}(\mathcal{H}_2,\mathcal{H}_3))$ and $\boldsymbol{B} \in S^{\omega_2}(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2))$ belongs to the symbol class $S^{\omega_1\omega_2}(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_3))$. Of special importance for the semiclassical symbol calculus and especially for SAPT is the so–called Weyl product which corresponds to the operator product of quantum operators underlying the Weyl quantization prescription.

Proposition 6.3. The Weyl Product
Let $\boldsymbol{A} \in S^{m_1}_\rho(\mathcal{B}(\mathcal{H}_2,\mathcal{H}_3))$ and $\boldsymbol{B} \in S^{m_2}_\rho(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2))$. Then the operator product $\hat{\boldsymbol{A}}\hat{\boldsymbol{B}}$ of their Weyl quantizations is well–defined and given by $\hat{\boldsymbol{A}}\hat{\boldsymbol{B}} = \hat{\boldsymbol{C}}$ with $\boldsymbol{C} \in S^{m_1+m_2}_\rho(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_3))$ of the form

$$\boldsymbol{C}(q,p) = \exp\left(\frac{i\varepsilon}{2}(\partial_q\partial_\xi - \partial_p\partial_x)\right)\boldsymbol{A}(q,p)\cdot\boldsymbol{B}(x,\xi)\Big|_{x=q,\xi=p} =: \boldsymbol{A}\,\tilde{\bigstar}_\varepsilon\,\boldsymbol{B}. \tag{6.46}$$

A similar result holds for the symbol classes S^{ω}. In particular, let $\boldsymbol{A} \in S^{\omega_1}(\mathcal{B}(\mathcal{H}_2,\mathcal{H}_3))$ and $\boldsymbol{B} \in S^{\omega_2}(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2))$. Then, we have $\hat{\boldsymbol{A}}\hat{\boldsymbol{B}} = \hat{\boldsymbol{C}}$ with $\boldsymbol{C} \in S^{\omega_1\omega_2}(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_3))$ where $\boldsymbol{C}(q,p)$ arises from (6.46).

Note that the symbol classes $S^0_\rho(\mathcal{B}(\mathcal{H}))$ and $S^\infty_\rho(\mathcal{B}(\mathcal{H})) := \bigcup_{m\in\mathbb{R}} S^m_\rho(\mathcal{B}(\mathcal{H}))$ are algebras with respect to the Weyl product $\tilde{\bigstar}_\varepsilon$. The form of the Weyl product as a power series in the perturbation parameter ε suggests to define classes of ε–dependent symbol functions. Suitably, these symbols correspond to power series in ε with coefficients in the classical symbol functions. The following definition of formal power series symbols proves to be useful.

Definition 6.4. Formal Power Series Symbols
Let $\{\boldsymbol{A}_j\}_{j\in\mathbb{N}}$ be a sequence of symbol functions with $\boldsymbol{A}_j \in S^\infty_\rho(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2))$ for every $j \in \mathbb{N}$. The subspace of the formal power series symbols is given by

$$M^m_\rho(\varepsilon,\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)) := \left\{\sum_{j\geq 0}\varepsilon^j\boldsymbol{A}_j \,:\, \boldsymbol{A}_j \in S^{m-j\rho}_\rho(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2))\right\}. \tag{6.47}$$

The formal power series symbols admit a star product which has the same form as the Weyl product in equation (6.46). However, this product is then referred to in the literature as the *Moyal*

product denoted by "$\star_\varepsilon$". The formal power series give rise to the following defintion of *(adiabatic) perturbation symbols*. We note that in the literature, these symbols are designated as "semiclassical symbols" (Teufel 2003, p. 209). This is reasonable in the respective cases where one considers the hypothetical limit $\hbar \to 0$. Here, we prefer to introduce the following terminology.

Definition 6.5. (Adiabatic) Perturbation Symbols
A map $\boldsymbol{A} : [0, \varepsilon_0) \to S^m_\rho(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)) : \varepsilon \mapsto \boldsymbol{A}_\varepsilon$ is an (adiabatic) perturbation symbol of order m and weight ρ if there exists a sequence $\{\boldsymbol{A}_j\}_{j\in\mathbb{N}}$ with $\boldsymbol{A}_j \in S^{m-j\rho}_\rho(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ (i.e., a formal power series symbol) such that for every $n \in \mathbb{N}$ and any $k \in \mathbb{N}$, there exists a constant $C_{n,k} > 0$ such that for any $\varepsilon \in [0, \varepsilon_0)$ one has

$$\left\| \boldsymbol{A}_\varepsilon - \sum_{j=0}^{n-1} \varepsilon^j \boldsymbol{A}_j \right\|_k^{(m-n\rho)} \leq C_{n,k}\, \varepsilon^n. \tag{6.48}$$

Here, $\|\cdot\|_k^{(m)}$ is the k^{th} Fréchet seminorm in $S^m_\rho(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$. It is also clear that then $\varepsilon^{-n}(\boldsymbol{A}_\varepsilon - \sum_{j=0}^{n-1} \varepsilon^j \boldsymbol{A}_j) \in S^{m-n\rho}_\rho$. We denote the space of these perturbation symbols of order m and weight ρ by $S^m_\rho(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ or simply as $S^m_\rho(\varepsilon)$. These definitions and all the following apply similarly to the symbol classes S^ω with generic order functions. If the series $\{\boldsymbol{A}_j\}_{j\in\mathbb{N}}$ satisfies condition (6.48) for some $\boldsymbol{A}_\varepsilon \in S^m_\rho(\varepsilon)$, one writes $\boldsymbol{A}_\varepsilon \asymp \sum_{j\geq 0} \varepsilon^j \boldsymbol{A}_j$, and we say that $\boldsymbol{A}_\varepsilon$ is asymptotically equivalent to the corresponding series expansion.

We emphasize that such a power series $\sum_{j\geq 0} \varepsilon^j \boldsymbol{A}_j$ need not always converge. However, it always corresponds to an asymptotic expansion of one (or several) adiabatic perturbation symbols $\boldsymbol{A}_\varepsilon$. Therefore, let us introduce the following notation.

Definition 6.6. The Error Estimate $\mathcal{O}(\varepsilon^\infty)$
If $\boldsymbol{A}_\varepsilon \asymp \sum_{j\geq 0} \varepsilon^j \boldsymbol{A}_j$ in $S^m_\rho(\varepsilon)$ and $\boldsymbol{A}_j = 0$ for every $j \in \mathbb{N}$, we write $\boldsymbol{A}_\varepsilon = \mathcal{O}(\varepsilon^\infty)$.

Then, we come back to the relation between the perturbation symbols $\boldsymbol{A}_\varepsilon$ and the formal power series $\sum_{j\in\mathbb{N}} \varepsilon^j \boldsymbol{A}_j$. In particular, we note that there exists a perturbation symbol $\boldsymbol{A}_\varepsilon \in S^m_\rho(\varepsilon)$ for *every* $\boldsymbol{A} \in M^m_\rho(\varepsilon, \mathcal{B}(\mathcal{H}))$ such that $\boldsymbol{A}_\varepsilon \asymp \sum_{j\geq 0} \varepsilon^j \boldsymbol{A}_j$, and $\boldsymbol{A}_\varepsilon = \boldsymbol{A}$ is unique up to $\mathcal{O}(\varepsilon^\infty)$. We then denote $\boldsymbol{A}_\varepsilon$ as a *resummation* of $\sum_{j\geq 0} \varepsilon^j \boldsymbol{A}_j$. It is important to realize that this notion of asymptotic equivalence can be weak for symbol classes with $\rho = 0$. For example, $\langle p\rangle^m e^{-1/\varepsilon} = \mathcal{O}(\varepsilon^\infty)$ in $S^m_0(\varepsilon)$. Therefore, it is reasonable to introduce a seperate, stronger statement for classes with $\rho > 0$.

Definition 6.7. Asymptotic Equivalence in $S^m_\rho(\varepsilon)$ for $\rho > 0$
For $\boldsymbol{A}_\varepsilon, \boldsymbol{B}_\varepsilon \in S^m_\rho(\varepsilon)$ with $\rho > 0$, we say that $\boldsymbol{B}_\varepsilon = \boldsymbol{A}_\varepsilon + \mathcal{O}_{-\infty}(\varepsilon^\infty)$ if $\boldsymbol{B}_\varepsilon - \boldsymbol{A}_\varepsilon = \mathcal{O}(\varepsilon^\infty)$ in $S^m_\rho(\varepsilon)$. Abusing the notation, one also writes $\hat{\boldsymbol{B}}_\varepsilon = \hat{\boldsymbol{A}}_\varepsilon + \mathcal{O}_{-\infty}(\varepsilon^\infty)$ if the corresponding symbols satisfy $\boldsymbol{B}_\varepsilon = \boldsymbol{A}_\varepsilon + \mathcal{O}_{-\infty}(\varepsilon^\infty)$.

Asymptotic equivalence for $\rho > 0$ is strong in the sense that there exist constants $C_{n,k} > 0$ for any $n, k \in \mathbb{N}$ such that $\|\boldsymbol{B}_\varepsilon - \boldsymbol{A}_\varepsilon\|_k^{(m-n\rho)} \leq C_{n,k}\varepsilon^n$ for any $\varepsilon \in [0, \varepsilon_0)$. Because $\rho > 0$, we have that $m - n\rho \geq 0$ for some $n \in \mathbb{N}$ and the theorem of Calderon–Vaillancourt assures that the difference operator $\hat{\boldsymbol{B}}_\varepsilon - \hat{\boldsymbol{A}}_\varepsilon$ is bounded in the $\mathcal{B}(L^2(\mathbb{R}, \mathcal{H}))$–norm. The statement can even be reinforced: $\hat{\boldsymbol{B}}_\varepsilon - \hat{\boldsymbol{A}}_\varepsilon$ is a smoothing operator, i.e., it belongs to $\mathrm{OPS}^{-\infty}_\rho := \bigcap_{m\in\mathbb{R}} \mathrm{OPS}^m_\rho$. In order to also have a weaker notion of an operator bound, we also introduce the $\mathcal{O}_0(\varepsilon^\infty)$ notation.

Definition 6.8. The Bound $\mathcal{O}_0(\varepsilon^\infty)$
Let $\hat{\boldsymbol{R}}_\varepsilon$ and $\hat{\boldsymbol{S}}_\varepsilon$ be two ε–dependent operators on $\mathcal{H}$. We say that $\hat{\boldsymbol{R}}_\varepsilon = \hat{\boldsymbol{S}}_\varepsilon + \mathcal{O}_0(\varepsilon^\infty)$ if for every $n \in \mathbb{N}$ there exists a constant $C_n > 0$ such that

$$\left\| \hat{\boldsymbol{R}}_\varepsilon - \hat{\boldsymbol{S}}_\varepsilon \right\|_{\mathcal{B}(L^2(\mathbb{R},\mathcal{H}_1),L^2(\mathbb{R},\mathcal{H}_2))} \leq C_n\, \varepsilon^n, \quad \forall \varepsilon \in [0, \varepsilon_0). \tag{6.49}$$

With these basic results (from (Teufel 2003)) regarding operator–valued pseudodifferential calculus, let us move on to its application to SAPT.

6.4. Space Adiabatic Perturbation Theory

In a nutshell, SAPT is a method to compute an improved Hamilton operator for a quantum system that includes the backreaction of an environment with a highly differing mass or energy scale. It thereby extends the standard Born–Oppenheimer theory to arbitrarily high orders in the perturbative scheme using the operator–valued pseudodifferential calculus of section 6.3. In this section, we present the conditions under which the theory applies (section 6.4.1), give an overview of the formalism (section 6.5), perform the iterative construction for arbitrary order (section 6.6), and give more details on the explicit construction up to second order that we use to derive our results within quantum cosmology (section 6.7). This section is mostly based and partially taken from the references (Schander and Thiemann 2019a,c), and which we will indicate in due course.

Similar to the former notation, we assume that the system of interest naturally splits into a slow subsystem with phase space variables (q, P) while the fast subsystem is labeled by the phase space variables (x, y). We consider a simple four–dimensional phase space $\Gamma = \Gamma_\mathrm{s} \times \Gamma_\mathrm{f} = \mathbb{R}^4$ where $\Gamma_\mathrm{s} = \mathbb{R}^2$ and $\Gamma_\mathrm{f} = \mathbb{R}^2$ denote the slow and the fast phase spaces respectively. A generalization to higher dimensional phase spaces proves to be straightforward (Teufel 2003). We also mention that to a certain extent it is also possible to generalize the scheme to finite dimensional phase spaces which are not vector spaces (Stottmeister and Thiemann 2016a,b,c), yet these are not of interest for our purposes. For the presented model, the phase space structure is provided by the only non–vanishing Poisson brackets $\{q, P\} = \{x, y\} = 1$. The classical Hamilton function specifying the dynamics of the theory will be denoted by $H(q, x, P, y)$ and is supposed to be a smooth function of the phase space variables.

SAPT is designed for the analysis of purely quantum mechanical systems, and again we label the operators associated with the slow subsystem by hats, for example $(\hat{q}, \hat{P})$ for the basic slow phase space operators. Bold letters stand for the operators of the fast subsystem, e.g., $(\boldsymbol{x}, \boldsymbol{y})$. We use the standard representation on the Hilbert space $\mathcal{H}_\mathrm{s} = L^2(\mathbb{R}, \mathrm{d}q)$ for the slow subsystem and similarly for the fast Hilbert space $\mathcal{H}_\mathrm{f} = L^2(\mathbb{R}, \mathrm{d}x)$. Position and momentum operators shall act in the standard way as multiplication and derivative operators on the respectively dense domains of definition in the Hilbert spaces. Position and momentum operator satisfy the commutation relations $[\hat{q}, \hat{P}] = i\,\hat{1}_\mathrm{s}$, and $[\boldsymbol{x}, \boldsymbol{y}] = i\mathbf{1}_\mathrm{f}$ respectively. The tensor product of these Hilbert spaces $\mathcal{H} := \mathcal{H}_\mathrm{f} \otimes \mathcal{H}_\mathrm{s}$ models the total Hilbert space of our system. The simplest form of a bounded operator acting on this Hilbert space would have the form of a topological tensor product $\hat{A} \otimes \boldsymbol{B}$ with $\hat{A} \in \mathcal{B}(\mathcal{H}_\mathrm{s})$ and $\boldsymbol{B} \in \mathcal{B}(\mathcal{H}_\mathrm{f})$. Every bounded operator ascends to an operator on the total Hilbert

space by tensor–multiplying with the respectively other unity operator. In order to make SAPT work at the technical level, the scheme resorts to a *phase space* or *deformation quantization* with respect to the slow subsystem while keeping the Hilbert space representation of the fast subsystem. Recall that this quantization scheme assigns a function on the slow phase space with values in the space of bounded operators on the fast Hilbert space to an appropriate classical observable, thus giving rise to the operator–valued pseudodifferential calculus of section 6.3. Besides, one performs an appropriate ε–scaling of the slow degrees of freedom. In the given cases, this amounts to defining the momentum $p := \varepsilon^k P$ with $k \in \mathbb{R}^+$. This gives rise to a modified commutation relation $[\hat{q}, \hat{p}] = i\varepsilon^k \hat{1}_s$ for the slow sector and to an ε–scaled pseudodifferential calculus. As in standard quantum theory, it is necessary to choose an ordering prescription for quantum operators and we will stick here to the symmetric Weyl ordering procedure, (B. C. Hall 2013, p. 261), although different orderings are conceivable (Blaszak and Domanski 2012, Section 3).

6.4.1. System Requirements

SAPT as introduced by Panati, Spohn, and Teufel (2003) places a set of restrictions on the physical system under consideration. These are, in some respects, quite restrictive. However, if one accepts to abandon certain results such as the convergence of the perturbative series, it is possible to milden the conditions. Here, we start by giving the original conditions by Panati, Spohn and Teufel, which can be split into four categories:

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

$$\mathcal{H} = L^2(\mathbb{R}) \otimes \mathcal{H}_f = L^2(\mathbb{R}, \mathcal{H}_f), \tag{6.50}$$

where $L^2(\mathbb{R})$ is the state space of the system whose rate of change is by a factor ε^k, $k \in \mathbb{R}^+$, smaller than the rate of change of the (environmental) system $\mathcal{H}_f$. The latter is assumed to be a separable Hilbert space.

(C2) **The quantum Hamiltonian $\hat{\boldsymbol{H}}$** (may it be an operator or a constraint) is given as the Weyl quantization of a semiclassical symbol $\boldsymbol{H} \in S^m_\rho(\varepsilon, \mathcal{B}(\mathcal{H}_f))$

$$\boldsymbol{H}(\varepsilon, z) \asymp \sum_{j=0}^{\infty} \varepsilon^j \boldsymbol{H}_j(z) \tag{6.51}$$

with values in the bounded self–adjoint operators on $\mathcal{H}_f$ where $z := (q, p) = (q, \varepsilon^k P)$.

(C3) For any fixed $z \in \mathbb{R}^2$, the spectrum $\sigma(z)$ of the principal symbol $\boldsymbol{H}_0(z)$ of $\boldsymbol{H}(\varepsilon, z)$ has at least one isolated part $\sigma_\nu(z)$ associated with a fixed quantum number $\nu \in \mathbb{N}$ of the fast system (see Figure 6.1). In particular, the minimal distance between the elements of $\sigma_\nu(z)$ and the remainder of the spectrum $\sigma_{\text{rem}}(z) := \sigma(z) \backslash \sigma_\nu(z)$ represent a non–vanishing gap. According to its characteristics with varying z, the gap can be classified by means of a parameter γ. **Conditions** $(\textbf{Gap})_\gamma$: Let $f_\pm \in C^0(\mathbb{R}^2, \mathbb{R})$ be two continuous functions with $f_- \leq f_+$.

(G1) **Enclosing interval.** For every $z \in \mathbb{R}^2$ the isolated part of the spectrum $\sigma_\nu(z)$ is entirely contained in the interval $I(z) := [f_-(z), f_+(z)]$.

(G2) **Gap to the remainder.** The distance between the remainder of the spectrum $\sigma_{\text{rem}}(z)$

and the enclosing interval $I(z)$ is strictly bigger than zero and increasing for large momenta, i.e.,

$$\mathrm{Dist}\left[\sigma_{\mathrm{rem}}(z), I(z)\right] \geq C_{\mathrm{g}}(1+p^2)^{\frac{\gamma}{2}}. \tag{6.52}$$

(G3) **Boundedness of the interval.** The width of the interval $I(z)$ is uniformly bounded, *i.e.*,

$$\sup_{z\in\mathbb{R}^2} |f_+(z) - f_-(z)| \leq C_{\mathrm{d}} < \infty. \tag{6.53}$$

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

We note that (C4) is not vital to perform the formal computations in the following. It ensures however that for considerations on the whole slow phase space $\mathbb{R}^2$, the error estimates of SAPT are bounded everywhere on $\mathbb{R}^2$. In particular, the adiabatic decoupling is said to be *uniform*.

The following figure shows a possible configuration of energy bands of the Hamilton symbol $\boldsymbol{H}(q,p)$. The relevant energy band (in purple) is separated by the two functions f_+ and f_- from the remainder of the spectrum (in green) everywhere on the phase space $\mathbb{R}^2$.

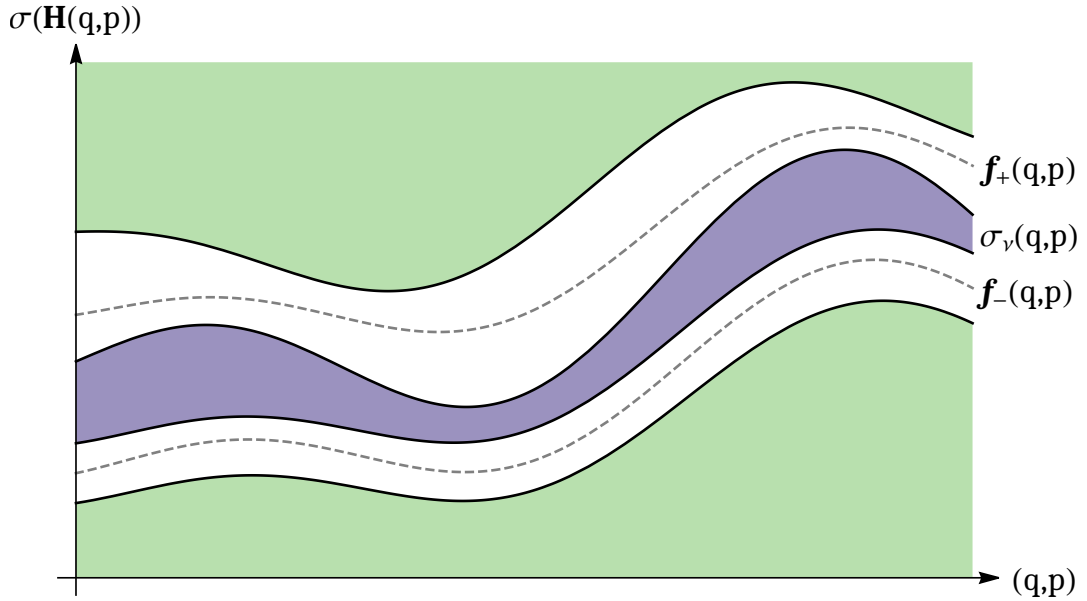

Figure 6.1.: Qualitative illustration of the spectrum of a symbol Hamiltonian with corresponding energy bands. The graphic is inspired by (Teufel 2003).

6.5. The Space Adiabatic Formalism

To explain the general idea of SAPT, let us assume that all four conditions (C1) – (C4) are satisfied. This means that we have a semiclassical Hamilton symbol $\boldsymbol{H}^m_\rho(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ with values in the bounded, self–adjoint operators and whose Weyl quantization is a well–defined operator on $\mathcal{H} = L^2(\mathbb{R}, \mathcal{H}_{\mathrm{f}})$. Its spectrum satisfies the gap condition for some $\gamma \in \mathbb{R}$ with $\gamma = m$ if $\rho > 0$ or if $\rho = 0$ also γ vanishes. Besides, let us choose one single energy band with fast quantum number

$\nu \in \mathbb{N}$ that will backreact on the slow subsystem. In the following, we discuss the scheme of SAPT in more detail splitting it into three stages. Note that a similar account of SAPT can also be found in (Schander and Thiemann 2019a) on which this section is based together with (Teufel 2003). Unless stated otherwise, the given results and many more details can be found in (Teufel 2003).

6.5.1. The Moyal Projector

The first step of the scheme consists in constructing an operator which is an almost projector and almost invariant under the dynamics of the total Hamiltonian $\hat{\boldsymbol{H}}$ where "almost" refers to an error of the desired order in ε. Therefore, consider the gap condition (C3) according to which the principal Hamilton symbol $\boldsymbol{H}_0(q,p)$ admits a pointwise separated energy band $E_\nu(q,p)$ associated with one of its (fast) quantum numbers $\nu \in \mathbb{N}$. The (q,p)–dependent eigensolution in $\mathcal{H}_\mathrm{f}$ is $\xi_\nu(q,p)$ with

$$\boldsymbol{H}_0(q,p)\,\xi_\nu(q,p) = E_\nu(q,p)\,\xi_\nu(q,p). \tag{6.54}$$

We assume that E_ν is a simple energy band without degeneracies although the extension to non–simple and degenerate energy bands is straightforward as long as the gap condition is satisfied. One can consider the eigenvalue equation (6.54) as a stationary quantum problem for *fixed* classical nuclei configurations $(q,p) \in \mathbb{R}^2$. The interesting question is how these stationary ansatz solutions evolve under the dynamics of the Hamilton operator $\hat{\boldsymbol{H}}$ and whether they provide an approximation to the solutions of the dynamical quantum problem. More precisely, does the ε–scaled Weyl quantization $\mathcal{W}_\varepsilon(\boldsymbol{\pi}_0)$ of the projection symbol $\boldsymbol{\pi}_0(q,p) := \xi_\nu(q,p)\,\langle \xi_\nu(q,p), \cdot\,\rangle_\mathrm{f}$ (where the angular brackets denote the inner product within $\mathcal{H}_\mathrm{f}$) approach a true dynamical projection operator $\hat{\boldsymbol{P}}$ of the Hamiltonian $\hat{\boldsymbol{H}}$, i.e., an operator $\hat{\boldsymbol{P}}$ which satisfies $[\hat{\boldsymbol{P}}, \hat{\boldsymbol{H}}] = 0$? The answer to this question is in the positive although $\boldsymbol{\pi}_0$ only provides a first order approximation with respect to ε. In particular, by pulling back the computations to phase space using the Weyl ordered phase space quantization scheme with the Moyal product $\star_\varepsilon$, it is easy to verify that

$$\boldsymbol{H} \star_\varepsilon \boldsymbol{\pi}_0 - \boldsymbol{\pi}_0 \star_\varepsilon \boldsymbol{H} \sim \varepsilon. \tag{6.55}$$

Besides, $\boldsymbol{\pi}_0$ also fails to provide an exact projection operator on the full Hilbert space. Instead, we have that $\boldsymbol{\pi}_0 \star_\varepsilon \boldsymbol{\pi}_0 - \boldsymbol{\pi}_0 \sim \varepsilon$. The space adiabatic theorem provides a mean to improve the situation (Teufel 2003). It states that if conditions (C1) – (C4) are fulfilled, there exists indeed an orthogonal projection operator $\hat{\boldsymbol{\Pi}} \in \mathcal{B}(\mathcal{H})$ on the total Hilbert space such that (Teufel 2003)

$$\big[\hat{\boldsymbol{H}}, \hat{\boldsymbol{\Pi}}\big] = \mathcal{O}_0(\varepsilon^\infty), \tag{6.56}$$

i.e., $\hat{\boldsymbol{\Pi}}$ approaches $\hat{\boldsymbol{P}}$ up to infinite order in ε, and most importantly, there exists an adiabatic symbol function $\boldsymbol{\pi}_\varepsilon \in S^0_\rho(\varepsilon)$ whose Weyl quantization gives rise to the construction of the above projection operator $\hat{\boldsymbol{\Pi}} = \hat{\mathcal{W}}_\varepsilon(\boldsymbol{\pi}_\varepsilon) + \mathcal{O}_0(\varepsilon^\infty)$. This relation can be established using resolvent methods (Nenciu and Sordoni 2001; Teufel 2003), and it assures that these operators are indeed very close in norm.

The idea of SAPT is to iteratively construct a Moyal projection symbol

$$\boldsymbol{\pi} := \sum_{i=0}^{\infty} \varepsilon^i \boldsymbol{\pi}_i \;\in S^0_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f})) \tag{6.57}$$

which takes $\boldsymbol{\pi}_0$ as its inductive starting point and for which $\boldsymbol{\pi}_\varepsilon$ is a suitable resummation. Note that $\boldsymbol{\pi}_0$ still depends on the fixed quantum number $\nu \in \mathbb{N}$, and so do the higher iterations $\boldsymbol{\pi}_i$ for every $i \in \mathbb{N}$. We will however not explicitely name this dependence here and in the following due to notational reasons.

The space adiabatic theorem assures that $\boldsymbol{\pi}_i$ is in the symbol class $S_\rho^{-i\rho}(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ for any $i \in \mathbb{N}$ due to the convergence condition (C4). In case of a convergent power series, we can simply identify $\boldsymbol{\pi}_\varepsilon$ with $\boldsymbol{\pi}$ but the results in Teufel (2003) include the divergent case for which the distinction becomes relevant. We would then have that $\boldsymbol{\pi}_\varepsilon = \boldsymbol{\pi} + \mathcal{O}_0(\varepsilon^\infty)$. In either case, we can relate the Weyl quantization of the symbol function $\boldsymbol{\pi}_\varepsilon$ to the projection operator $\hat{\boldsymbol{\Pi}}$ according to the space adiabatic theorem. According to the latter, the properties of $\boldsymbol{\pi}$ are naturally given as

$$\text{(S1–1)}\, \boldsymbol{\pi} \star_\varepsilon \boldsymbol{\pi} = \boldsymbol{\pi}, \quad \text{(S1–2)}\, \boldsymbol{\pi}^* = \boldsymbol{\pi}, \quad \text{(S1–3)}\, \boldsymbol{H} \star_\varepsilon \boldsymbol{\pi} - \boldsymbol{\pi} \star_\varepsilon \boldsymbol{H} = 0, \tag{6.58}$$

and these relations serve to define an iterative procedure for the construction of $\boldsymbol{\pi}$ by means of the ε–dependent Moyal star product $\star_\varepsilon$. The Weyl quantization $\hat{\boldsymbol{\pi}}_\varepsilon$ is a bounded operator on $\mathcal{H}$ due to the theoreom of Calderon–Vaillancourt and the fact that $\boldsymbol{\pi} \in S_\rho^0$. In particular, it holds true that

$$\text{(S1–1)'}\, \hat{\boldsymbol{\pi}}_\varepsilon^2 = \hat{\boldsymbol{\pi}}_\varepsilon + \mathcal{O}_{-\infty}(\varepsilon^\infty), \quad \text{(S1–2)'}\, \hat{\boldsymbol{\pi}}_\varepsilon^\dagger = \hat{\boldsymbol{\pi}}_\varepsilon, \quad \text{(S1–3)'}\, \hat{\boldsymbol{H}}\, \hat{\boldsymbol{\pi}}_\varepsilon - \hat{\boldsymbol{\pi}}_\varepsilon \hat{\boldsymbol{H}} = \mathcal{O}_{-\infty}(\varepsilon^\infty). \tag{6.59}$$

If $\hat{\boldsymbol{H}}$ is unbounded but has a symbol $\boldsymbol{H}$ in S_ρ^m with $m > 0$ and $\rho > 0$, the latter equality holds in the norm of bounded operators. However, if $\rho = 0$ while $m > 0$, this is not true anymore. The convergence condition (C4) is crucial for the results (6.59) to be valid as otherwise one cannot assume that $\boldsymbol{\pi}$ gives rise to a bounded operator on $\mathcal{H}$. We refer to Teufel (2003, p. 80 ff.) for the explicit proof of these statements. For a convergent series $\boldsymbol{\pi} = \boldsymbol{\pi}_\varepsilon$, one can omit the above error terms. In the divergent case, the true projection operator $\hat{\boldsymbol{\Pi}}$ emerges from $\hat{\boldsymbol{\pi}}_\varepsilon$ using resolvent methods.

In the next step, one would like to restrict the Hamiltonian to the single subspace associated with $\hat{\boldsymbol{\Pi}}$. Intuitively, the dynamics of $\hat{\boldsymbol{\Pi}}\hat{\boldsymbol{H}}\hat{\boldsymbol{\Pi}}$ should be trivial as we already know the solutions of the fast subsystem ξ_ν. There are however problems with using $\hat{\boldsymbol{\Pi}}$ directly. First, the limit $\lim_{\varepsilon\to 0}\hat{\boldsymbol{\Pi}}$ does not exist. As a consequence, $\hat{\boldsymbol{\Pi}}\mathcal{H}$ might not even be close to an ε–independent subspace, and the entire scheme would depend heavily on the specific value of ε. Note also that an analysis of the subspace $\hat{\boldsymbol{\Pi}}\mathcal{H}$ turns out to be a difficult or even impossible task because $\boldsymbol{\pi}$ depends very non–trivially on the slow phase space variables. Besides, it turns out that for any $I < \infty$, the Weyl quantization $\hat{\boldsymbol{\pi}}_{(I)}$ of the projector symbol function

$$\boldsymbol{\pi}_{(I)} := \sum_{i=0}^{I} \varepsilon^i \boldsymbol{\pi}_i \tag{6.60}$$

is by construction *not* an exact projector on the total Hilbert space $\mathcal{H}$ (Schander and Thiemann 2019a). In particular, the restricted operator $\hat{\boldsymbol{H}}|_{\hat{\boldsymbol{\pi}}_{(I)}} := \hat{\boldsymbol{\pi}}_{(I)}\hat{\boldsymbol{H}}\hat{\boldsymbol{\pi}}_{(I)}$ does *not* preserve the subspace $\hat{\boldsymbol{\pi}}_{(I)}\mathcal{H}$. As a consequence, it remains unclear how to perform a spectral analysis for this operator on $\hat{\boldsymbol{\pi}}_{(I)}\mathcal{H} \subset \mathcal{H}$. Even worse, the operator $\hat{\boldsymbol{H}}|_{\hat{\boldsymbol{\pi}}_{(I)}}$ maps states in $\hat{\boldsymbol{\pi}}_{(I)}\mathcal{H}$ outside of this domain. SAPT resorts therefore to a suitable reference space that does neither depend on ε nor on the slow phase space variables.

6.5.2. The Moyal Unitary

Consider a symbol function $\boldsymbol{u}_0(q,p)$ which maps the subspace $\boldsymbol{\pi}_0\mathcal{H}_\mathrm{f} \subset \mathcal{H}_\mathrm{f}$ to a (q,p)–*independent* subspace of $\mathcal{H}_\mathrm{f}$. A simple proposal for this is the following: Fix a specific point in the slow phase space $(q_0,p_0) \in \mathbb{R}^2$. The choice can be physically motivated and depends on the problem under consideration. Take the eigenbasis $\{\xi_n(q,p)\}_n$ associated with $\boldsymbol{H}_0(q,p)$, and denote the basis at the point (q_0,p_0) by $\{\zeta\}_n := \{\xi_n(q_0,p_0)\}_n$. This motivates the definition of the unitary symbol

$$\boldsymbol{u}_0(q,p) := \sum_{n=0}^{\infty} \zeta_n \langle \xi_n(q,p), \cdot \rangle_\mathrm{f} \tag{6.61}$$

where we assume that none of the eigenstates is degenerate. Of course, the $\{\zeta_n\}_n$ could be any orthonormal basis of $\mathcal{H}_\mathrm{f}$. The important point is that the reference vectors ζ_n do *not* depend on (q,p). One can then define the reference projection associated with the quantum number ν as above according to

$$\boldsymbol{\pi}_\mathrm{R} := \zeta_\nu \langle \zeta_\nu, \cdot \rangle_\mathrm{f}. \tag{6.62}$$

The technical relevance of this reference structure is that $\boldsymbol{\pi}_\mathrm{R}$, in contrast to $\boldsymbol{\pi}_0$, does not receive adiabatic corrections throughout the application of the space adiabatic perturbation scheme, and thus, always defines an *exact* projector on the total Hilbert space by

$$\hat{\boldsymbol{\pi}}_\mathrm{R} = \hat{\mathcal{W}}(\hat{\boldsymbol{\pi}}_\mathrm{R}) = \boldsymbol{\pi}_\mathrm{R} \otimes \hat{1}_\mathrm{s}. \tag{6.63}$$

Formally, the scheme then constructs the Moyal unitary $\boldsymbol{u}(q,p)$ as a power series in ε according to

$$\boldsymbol{u}(q,p) = \sum_{i=0}^{\infty} \varepsilon^i \boldsymbol{u}_i(q,p) \tag{6.64}$$

with the symbol $\boldsymbol{u}_0$ in equation (6.61) as a starting point. It is easy to verify that $\boldsymbol{u}_0$ indeed intertwines the symbols $\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}_\mathrm{R}$ according to $\boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}_0^* = \boldsymbol{\pi}_\mathrm{R}$ where the dot denotes the operator product within the fast quantum algebra. The scheme then assures the existence of the Moyal unitary $\boldsymbol{u}$ in (6.64) which satisfies the following equalities:

$$\text{(S2–1)}\, \boldsymbol{u}^* \star_\varepsilon \boldsymbol{u} = \mathbf{1}_\mathrm{f}, \quad \text{(S2–2)}\, \boldsymbol{u} \star_\varepsilon \boldsymbol{u}^* = \mathbf{1}_\mathrm{f}, \quad \text{(S2–3)}\, \boldsymbol{u} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{u}^* = \boldsymbol{\pi}_\mathrm{R}. \tag{6.65}$$

These equations give rise to a series of algebraic equations which determine $\boldsymbol{u}_i \in S^{-i\rho}_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ for every $i \in \mathbb{N}$ order by order in ε. Let us assume that it is possible to establish the whole series $\sum_{i\geq 0} \varepsilon^i \boldsymbol{u}_i$. Then, there exists a(n up to terms of order $\mathcal{O}_{-\infty}(\varepsilon^\infty)$) unique resummation $\boldsymbol{u}_\varepsilon$ of $\boldsymbol{u} \in S^0_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ whose Weyl quantization $\hat{\boldsymbol{u}}_\varepsilon$ is a bounded operator on $\mathcal{H}$ satisfying

$$\text{(S2–1)'}\ \hat{\boldsymbol{u}}_\varepsilon^\dagger \hat{\boldsymbol{u}}_\varepsilon = \hat{\mathbf{1}} + \mathcal{O}_{-\infty}(\varepsilon^\infty), \tag{6.66}$$

$$\text{(S2–2)'}\ \hat{\boldsymbol{u}}_\varepsilon \hat{\boldsymbol{u}}_\varepsilon^\dagger = \hat{\mathbf{1}} + \mathcal{O}_{-\infty}(\varepsilon^\infty), \tag{6.67}$$

$$\text{(S2–1)'}\ \hat{\boldsymbol{u}}_\varepsilon \hat{\boldsymbol{\pi}}_\varepsilon \hat{\boldsymbol{u}}_\varepsilon^\dagger = \hat{\boldsymbol{\pi}}_\mathrm{R} + \mathcal{O}_{-\infty}(\varepsilon^\infty) \tag{6.68}$$

where $\hat{\mathbf{1}}$ is the unity operator associated with the entire system. Obviously, the resummation operator $\hat{\boldsymbol{u}}_\varepsilon$ is only almost unitary and intertwines $\hat{\boldsymbol{\pi}}_\varepsilon$ and $\hat{\boldsymbol{\pi}}_\mathrm{R}$ only up to some ε–dependent error. It is however possible to modify $\hat{\boldsymbol{u}}_\varepsilon$ by a term in $\mathcal{O}_0(\varepsilon^\infty)$ which makes it a true unitary operator $\hat{\boldsymbol{U}}$.

Moreover, this operator turns out to be a true intertwining operator in the sense that $\hat{\boldsymbol{U}}\,\hat{\boldsymbol{\Pi}}\,\hat{\boldsymbol{U}}^\dagger = \hat{\boldsymbol{\pi}}_{\mathrm{R}}$.

As for the Moyal projector, we will restrict ourselves to determine the Moyal unitary up to some finite order $I \in \mathbb{N}$ given by

$$\boldsymbol{u}_{(I)} = \sum_{i=0}^{I} \varepsilon^i \boldsymbol{u}_i. \tag{6.69}$$

The Moyal projector and the Moyal unitary allow to map the dynamics of $\hat{\boldsymbol{H}}$ to the reference space associated with $\hat{\boldsymbol{\pi}}_{\mathrm{R}}$ which gives rise to a new effective and much simpler Hamiltonian.

6.5.3. The Effective Hamiltonian

The effective Hamiltonian corresponds to the unitary transformation of the original Hamiltonian $\hat{\boldsymbol{H}}$ to the simple reference space, and thus provides the possibility to qualitatively derive the dynamics of the system on the reference space. The effective Hamiltonian symbol is defined as

$$\text{(S3)}\ \ \boldsymbol{h}_{\mathrm{eff}} := \boldsymbol{u} \star_\varepsilon \boldsymbol{H} \star_\varepsilon \boldsymbol{u}^*. \tag{6.70}$$

We denote the Weyl quantization of its resummation by $\hat{\boldsymbol{h}}_{\mathrm{eff},\varepsilon}$. The corresponding symbol function $\boldsymbol{h}_{\mathrm{eff},\varepsilon}(q,p)$ is a semiclassical symbol in $S^m_\rho(\varepsilon)$ since $\boldsymbol{u} \in S^0_\rho(\varepsilon)$ and $\boldsymbol{H} \in S^\rho_m(\varepsilon)$. Note that $\hat{\boldsymbol{h}}_{\mathrm{eff},\varepsilon}$ is in fact essentially self–adjoint on the Schwartz space $\mathcal{S}(\mathbb{R}, \mathcal{H}_{\mathrm{f}})$ (Teufel 2003). It generates an evolution very close to the original Hamilton operator namely

$$e^{-i\hat{\boldsymbol{H}}s} - \hat{\boldsymbol{u}}_\varepsilon^\dagger\, e^{-i\hat{\boldsymbol{h}}_{\mathrm{eff},\varepsilon}s}\,\hat{\boldsymbol{u}}_\varepsilon = \mathcal{O}_0(\varepsilon^\infty|s|). \tag{6.71}$$

To further simplify the computations, one can consider the effective Hamiltonian restricted to the reference space, i.e., the symbol $\boldsymbol{\pi}_{\mathrm{R}}\,\boldsymbol{h}_{\mathrm{eff}}\,\boldsymbol{\pi}_{\mathrm{R}}$ instead of $\boldsymbol{h}_{\mathrm{eff}}$. This makes sense since the construction scheme for $\hat{\boldsymbol{u}}$ guarantees that $\boldsymbol{h}_{\mathrm{eff}}$ preserves the subspace $\hat{\boldsymbol{\pi}}_{\mathrm{R}}\mathcal{H}$. As also discussed in (Schander and Thiemann 2019a), the subsequent applications, this statement translates into the assertion that the reduced operator $\hat{\boldsymbol{h}}_{\mathrm{eff},(I)} := \hat{\boldsymbol{u}}_{(I)}\hat{\boldsymbol{H}}\,\hat{\boldsymbol{u}}_{(I)}^\dagger$ preserves the subspace $\hat{\boldsymbol{\pi}}_{\mathrm{R}}\mathcal{H}$ up to corrections of order ε^{I+1}. It thus coincides up to corrections of order ε^{I+1} with the operator $\hat{\boldsymbol{h}}_{\mathrm{eff},(I),\mathrm{R}} := \hat{\boldsymbol{\pi}}_{\mathrm{R}}\,\hat{\boldsymbol{u}}_{(I)}\,\hat{\boldsymbol{H}}\,\hat{\boldsymbol{u}}_{(I)}^\dagger\,\hat{\boldsymbol{\pi}}_{\mathrm{R}}$ on the Hilbert subspace $\hat{\boldsymbol{\pi}}_{\mathrm{R}}\mathcal{H} \cong \mathcal{H}_{\mathrm{s}} \otimes \mathbb{C}$. The seemingly more natural operator $\hat{\boldsymbol{\pi}}_{(I)}\,\hat{\boldsymbol{H}}\,\hat{\boldsymbol{\pi}}_{(I)}$ does not preserve the subspace $\hat{\boldsymbol{\pi}}_{(I)}\mathcal{H}$ because $\hat{\boldsymbol{\pi}}_{(I)}$ is not an exact projector. As a result, $\hat{\boldsymbol{h}}_{\mathrm{eff},(I),\mathrm{R}}$ provides the perturbative adiabatic decoupling that we wanted to achieve, and will consequently be the object of interest in the sequel.

The spectrum of $\hat{\boldsymbol{h}}_{\mathrm{eff},(I),\mathrm{R}}$, denoted by $E_{\mathrm{eff},(I)}$ is referrred to as the ν–th energy band (recall that we restricted the backreactions to the fast quantum number ν right from the beginning). If $\Psi_{(I),\nu,\lambda}$ is a generalized eigenvector of $\hat{\boldsymbol{h}}_{\mathrm{eff},(I),\mathrm{R}}$ with eigenvalue λ then up to corrections of order ε^{I+1}, the vector $\tilde{\Psi}_{(I),\nu,\lambda} = \hat{\boldsymbol{u}}_{(I)}^\dagger \Psi_{(I),\nu,\lambda}$ is a generalized eigenvector of the orginal Hamiltonian $\hat{\boldsymbol{H}}$ with the same eigenvalue λ (Schander and Thiemann 2019a): This can be easily reproduced, dropping any contributions of order $\mathcal{O}(\varepsilon^{I+1})$, such that

$$\begin{aligned}\hat{\boldsymbol{H}}\tilde{\Psi}_{(I),\nu,\lambda} &= \hat{\boldsymbol{H}}\,\hat{\boldsymbol{u}}_{(I)}^\dagger\hat{\boldsymbol{\pi}}_{\mathrm{R}}\,\hat{\boldsymbol{u}}_{(I)}\hat{\boldsymbol{u}}_{(I)}^\dagger\Psi_{(I),\nu,\lambda} = \hat{\boldsymbol{H}}\,\hat{\boldsymbol{\pi}}_{(I)}\hat{\boldsymbol{u}}_{(I)}^\dagger\Psi_{(I),\nu,\lambda} = \hat{\boldsymbol{\pi}}_{(I)}\hat{\boldsymbol{H}}\,\hat{\boldsymbol{u}}_{(I)}^\dagger\Psi_{(I),\nu,\lambda}\\ &= \hat{\boldsymbol{u}}_{(I)}^\dagger(\hat{\boldsymbol{\pi}}_{\mathrm{R}}\,\hat{\boldsymbol{u}}_{(I)}\hat{\boldsymbol{H}}\hat{\boldsymbol{u}}_{(I)}^\dagger\hat{\boldsymbol{\pi}}_{(I)})\Psi_{(I),\nu,\lambda} = \hat{\boldsymbol{u}}_{(I)}^\dagger\hat{\boldsymbol{h}}_{\mathrm{eff},(I),\mathrm{R}}\Psi_{(I),\nu,\lambda} = \lambda\,\tilde{\Psi}_{(I),\nu,\lambda}.\end{aligned} \tag{6.72}$$

The approximate eigenvector $\tilde{\Psi}_{(I),\nu,\lambda}$ is an element of the approximately invariant subspace $\hat{\boldsymbol{\pi}}_{(I)}\mathcal{H}$ up to corrections of order $\mathcal{O}(\varepsilon^{I+1})$

$$\tilde{\Psi}_{(I),\nu,\lambda} = \hat{\boldsymbol{u}}^{\dagger}_{(I)}\hat{\boldsymbol{\pi}}_{\mathrm{R}}\,\hat{\boldsymbol{u}}_{(I)}\hat{\boldsymbol{u}}^{\dagger}_{(I)}\Psi_{(I),\nu,\lambda} = \hat{\boldsymbol{\pi}}_{(I)}\tilde{\Psi}_{(I),\nu,\lambda}. \tag{6.73}$$

As already discussed in (Schander and Thiemann 2019a), the $\hat{\boldsymbol{u}}_{(I)}$ are displayed as an auxiliary structure introduced in order to solve the spectral problem including backreations. But they have no further fundamental relevance as is also clear from the fact that they are not uniquely determined by the perturbative scheme. Besides, we note that $\hat{\boldsymbol{u}}_{(I)}$ is not to be confused with the unitary map $\hat{\boldsymbol{V}}$ that maps $\mathcal{H}$ to $L^2(\sigma(\hat{\boldsymbol{H}}), \mathrm{d}\mu)$, granted to exist by the spectral theorem, where $\sigma(\hat{\boldsymbol{H}})$ is the spectrum of $\hat{\boldsymbol{H}}$ and μ its spectral measure. This is already clear from the fact that $\hat{\boldsymbol{u}}_{(I)}$ generically depends on ν while $\hat{\boldsymbol{V}}$ does not. The fact that the $\hat{\boldsymbol{\pi}}_{(I)}$ approximately commute with $\hat{\boldsymbol{H}}$ and are approximate projections displays them as approximants of spectral projections of $\hat{\boldsymbol{H}}$ on the part $E_{\mathrm{eff},(I)}$ of the spectrum. The spectral projections are of course not necessarily mutually orthogonal even if the gap condition holds (unless the energy bands are strictly mutually disjoint). For instance, $\boldsymbol{H}(q,p)$ could have pure point spectrum but $\hat{\boldsymbol{H}}$ could have absolutely continuous spectrum.

We summarize the formalism for a system with Hamilton symbol $\boldsymbol{H} \in S^m_\rho$. If the system satisfies the conditions (C1) – (C4), the space adiabatic theorem assures that:

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

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

It can be shown that the Weyl quantization of a resummation of $\boldsymbol{\pi}$ which we denote by $\boldsymbol{\pi}_\varepsilon$ is $\mathcal{O}_0(\varepsilon^\infty)$–close to an operator $\hat{\boldsymbol{\Pi}}$, i.e., $\hat{\boldsymbol{\Pi}} = \hat{\boldsymbol{\pi}}_\varepsilon + \mathcal{O}_0(\varepsilon^\infty)$ and that $[\hat{\boldsymbol{H}}, \hat{\boldsymbol{\Pi}}] = \mathcal{O}_0(\varepsilon^\infty)$ (Teufel 2003, p. 75). Hence, the symbol function $\boldsymbol{\pi}$ gives indeed rise to an (almost) projector onto one of the dynamical subspaces of $\hat{\boldsymbol{H}}$.

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

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

The Weyl quantization of a resummation of $\boldsymbol{u}$ which we denote by $\boldsymbol{u}_\varepsilon$ gives rise to an operator $\hat{\boldsymbol{U}} = \hat{\boldsymbol{u}}_\varepsilon + \mathcal{O}_0(\varepsilon^\infty)$ for which it holds true that $\hat{\boldsymbol{U}}\,\hat{\boldsymbol{\Pi}}\,\hat{\boldsymbol{U}}^\dagger = \hat{\boldsymbol{\pi}}_{\mathrm{R}}$ (Teufel 2003, p. 85).

(S3) There exists a formal effective Hamilton symbol $\boldsymbol{h}_{\mathrm{eff}} = \sum_{i\geq 0}\varepsilon^i\boldsymbol{h}_{\mathrm{eff},i}$ defined as

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

For systems with an external time parameter t and the Weyl quantizations $\hat{\boldsymbol{u}}$ and $\hat{\boldsymbol{h}}_{\mathrm{eff}}$, we have (Teufel 2003, p. 90)

$$e^{-i\hat{\boldsymbol{H}}s} - \hat{\boldsymbol{u}}^\dagger e^{-i\hat{\boldsymbol{h}}_{\mathrm{eff}}s}\,\hat{\boldsymbol{u}} = \mathcal{O}_0(\varepsilon^\infty|s|). \tag{6.74}$$

6.6. Iterative Constructions

This section examines the iterative construction of the above symbol functions up to some arbitrary but finite order $I \in \mathbb{N}$. It is based and mostly taken from (Schander and Thiemann 2019a). The construction is founded on the assumption that the Moyal projector $\boldsymbol{\pi}(q,p)$, the Moyal unitary $\boldsymbol{u}(q,p)$, and the effective Hamilton symbol $\boldsymbol{h}_{\text{eff}}(q,p)$ appear as power series with respect to the adiabatic perturbation parameter ε, and we are going to concentrate on the determination of the power series coefficients up to this finite order $I \in \mathbb{N}$. I.e., we establish the symbols, $\boldsymbol{\pi}_{(I)} = \sum_{i\leq I} \varepsilon^i \boldsymbol{\pi}_i$, $\boldsymbol{u}_{(I)} = \sum_{i\leq I} \varepsilon^i \boldsymbol{u}_i$, and $\boldsymbol{h}_{\text{eff},(I)} = \sum_{i\leq I} \varepsilon^i \boldsymbol{h}_{\text{eff},i}$. Based on the construction rules (S1), (S2), and (S3), we can spell out the algebraic equations for determining any of the coefficients up to order $I \in \mathbb{N}$, in particular for the Moyal projector $\boldsymbol{\pi}$ these equations read

$$\begin{aligned}
&\text{(S1–1)''} \quad \boldsymbol{\pi}_{(I)} \star_\varepsilon \boldsymbol{\pi}_{(I)} - \boldsymbol{\pi}_{(I)} = \mathcal{O}_0(\varepsilon^{I+1}),\\
&\text{(S1–2)''} \quad \boldsymbol{\pi}^*_{(I)} - \boldsymbol{\pi}_{(I)} = \mathcal{O}_0(\varepsilon^{I+1}),\\
&\text{(S1–3)''} \quad \boldsymbol{H} \star_\varepsilon \boldsymbol{\pi}_{(I)} - \boldsymbol{\pi}_{(I)} \star_\varepsilon \boldsymbol{H} = \mathcal{O}_0(\varepsilon^{I+1}),
\end{aligned}$$

for the Moyal unitary $\boldsymbol{u}$ they are given by

$$\begin{aligned}
&\text{(S2–1)''} \quad \boldsymbol{u}^*_{(I)} \star_\varepsilon \boldsymbol{u}_{(I)} - \mathbf{1}_{\text{f}} = \mathcal{O}_0(\varepsilon^{I+1}),\\
&\text{(S2–2)''} \quad \boldsymbol{u}_{(I)} \star_\varepsilon \boldsymbol{u}^*_{(I)} - \mathbf{1}_{\text{f}} = \mathcal{O}_0(\varepsilon^{I+1}),\\
&\text{(S2–3)''} \quad \boldsymbol{u}_{(I)} \star_\varepsilon \boldsymbol{\pi}_{(I)} \star_\varepsilon \boldsymbol{u}^*_{(I)} - \boldsymbol{\pi}_{\text{R}} = \mathcal{O}_0(\varepsilon^{I+1}),
\end{aligned}$$

and for the effective Hamiltonian $\boldsymbol{h}_{\text{eff}}$ we finally have

$$\text{(S3)''} \quad \boldsymbol{h}_{\text{eff},(I)} - \boldsymbol{u}_{(I)} \star_\varepsilon \boldsymbol{H} \star_\varepsilon \boldsymbol{u}^*_{(I)} = \mathcal{O}_0(\varepsilon^{I+1}).$$

Regarding the $\mathcal{O}_0(\varepsilon^{I+1})$–estimate, we note that the space adiabatic theory assures that the symbol coefficients $\boldsymbol{\pi}_I$, $\boldsymbol{u}_I$ and $\boldsymbol{h}_{\text{eff},I}$ can be build in such a way that the coefficients of order ε^I and smaller vanish on the right hand sides of these equations. Besides, the product rule for semiclassical symbols assures that by plugging in the corresponding series expansions up to order I on the left hand side, the right hand sides will be symbols in the class $S^0_\rho(\mathcal{B}(\mathcal{H}_{\text{f}}))$ at most and so evaluate to bounded operators on the total Hilbert space. In equation (S3), this necessarily requires $\boldsymbol{H}$ to be in S^m_ρ with ρ strictly bigger than zero. In the following subsections, we provide the inductive construction rules for $\boldsymbol{\pi}_{(I)}$, $\boldsymbol{u}_{(I)}$ and $\boldsymbol{h}_{\text{eff},(I)}$, and therefore recall that the Moyal product for two symbols $\boldsymbol{B} \in S^{m_1}_\rho, \boldsymbol{C} \in S^{m_2}_\rho$ is given at leading order by

$$(\boldsymbol{B} \star_\varepsilon \boldsymbol{C})(q,p) = \boldsymbol{B}(q,p) \cdot \boldsymbol{C}(q,p) + \mathcal{O}_0(\varepsilon) \tag{6.75}$$

where $\mathcal{O}_0(\varepsilon)$ indicates that the remaining terms of this equation are of higher orders in ε.

6.6.1. Construction of the Moyal Projector

Based on the construction rules (S1)'', the Moyal projection symbol is to be determined iteratively up to order I. Therefore, the symbol function $\boldsymbol{\pi}_0(q,p)$ serves as the starting point for the induction

scheme. The expansion of the Moyal product in (S1)" simply gives the standard operator product on $\mathcal{B}(\mathcal{H}_\mathrm{f})$ at zeroth order such that its restriction to zeroth order yields

$$\text{(S1–1)}\,\boldsymbol{\pi}_0^2-\boldsymbol{\pi}_0=0,\quad \text{(S1–2)}\,\boldsymbol{\pi}_0^*-\boldsymbol{\pi}_0=0,\quad \text{(S1–3)}\,[\boldsymbol{H}_0,\boldsymbol{\pi}_0]_\mathrm{f}=0 \tag{6.76}$$

where the f–indexed brackets denote the commutator with respect to the fast operator algebra only. These equations are fulfilled by construction for $\boldsymbol{\pi}_0$ such that the basis case is granted. Let us then assume that it is possible to construct $\boldsymbol{\pi}_{(I-1)}$ and turn to the solution of the coefficient $\boldsymbol{\pi}_I$. The construction rule (S1–1)" provides the diagonal parts of $\boldsymbol{\pi}_I$. The induction scheme allows to assume that we already found $\boldsymbol{\pi}_{(I-1)}$ such that $\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\boldsymbol{\pi}_{(I-1)}-\boldsymbol{\pi}_{(I-1)}=\mathcal{O}_0(\varepsilon^I)$ is satisfied. We then denote the terms of (S1–1)" at order ε^I which only include the already known symbols $\boldsymbol{\pi}_{(I-1)}$ by $\boldsymbol{a}_{I-1}$. We then have that $\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\boldsymbol{\pi}_{(I-1)}-\boldsymbol{\pi}_{(I-1)}=:\ \varepsilon^I\boldsymbol{a}_{I-1}+\mathcal{O}_0(\varepsilon^{I+1})$. Importantly, $\boldsymbol{a}_{I-1}$ is already explicitely determined because of the induction assumption. For the induction step, we then consider the rule (S1–1)" *including* the symbol $\boldsymbol{\pi}_I$. By carrying all the terms with ε's of order $I+1$ and higher to $\mathcal{O}_0(\varepsilon^{I+1})$, (S1–1)" takes the form

$$\begin{aligned}\mathcal{O}_0(\varepsilon^{I+1})&=\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\boldsymbol{\pi}_{(I-1)}-\boldsymbol{\pi}_{(I-1)}+\varepsilon^I\boldsymbol{\pi}_I\cdot\boldsymbol{\pi}_0+\varepsilon^I\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_I-\varepsilon^I\boldsymbol{\pi}_I\\&=\varepsilon^I(\boldsymbol{a}_{I-1}+\boldsymbol{\pi}_I\cdot\boldsymbol{\pi}_0+\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_I-\boldsymbol{\pi}_I).\end{aligned} \tag{6.77}$$

To extract $\boldsymbol{\pi}_I$, we first define the orthogonal complement of $\boldsymbol{\pi}_0$ in $\mathcal{H}_\mathrm{f}$ as $\boldsymbol{\pi}_0^\perp:=\mathbf{1}_\mathrm{f}-\boldsymbol{\pi}_0$. Then, projecting (6.77) to the block diagonal pieces yields indeed the determining equations for the diagonal parts of $\boldsymbol{\pi}_I$ defined as

$$\boldsymbol{\pi}_I^{\mathrm{D},0}:=\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_I\cdot\boldsymbol{\pi}_0=-\boldsymbol{\pi}_0\cdot\boldsymbol{a}_{I-1}\cdot\boldsymbol{\pi}_0,\qquad \boldsymbol{\pi}_I^{\mathrm{D},\perp}:=\boldsymbol{\pi}_0^\perp\cdot\boldsymbol{\pi}_I\cdot\boldsymbol{\pi}_0^\perp=\boldsymbol{\pi}_0^\perp\cdot\boldsymbol{a}_{I-1}\cdot\boldsymbol{\pi}_0^\perp. \tag{6.78}$$

For the projection on the off–diagonal parts of $\boldsymbol{\pi}_I$, the consistency conditions

$$\boldsymbol{\pi}_0\cdot\boldsymbol{a}_{I-1}\cdot\boldsymbol{\pi}_0^\perp=0=\boldsymbol{\pi}_0^\perp\cdot\boldsymbol{a}_{I-1}\cdot\boldsymbol{\pi}_0 \tag{6.79}$$

arise. This identity follows from the defining equation (S1–1)" by projecting on the off–diagonal pieces and pushing all terms of order ε^{I+1} and higher into the error term. Furthermore, the associativity of the star product can be exploited to obtain

$$\begin{aligned}\varepsilon^I\boldsymbol{\pi}_0\cdot\boldsymbol{a}_{I-1}\cdot\boldsymbol{\pi}_0^\perp&=\boldsymbol{\pi}_0\cdot\big(\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\boldsymbol{\pi}_{(I-1)}-\boldsymbol{\pi}_{(I-1)}\big)\cdot\boldsymbol{\pi}_0^\perp+\mathcal{O}_0(\varepsilon^{I+1})\\&=\boldsymbol{\pi}_{(I-1)}\cdot\big(\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\boldsymbol{\pi}_{(I-1)}-\boldsymbol{\pi}_{(I-1)}\big)\cdot\boldsymbol{\pi}_{(I-1)}^\perp+\mathcal{O}_0(\varepsilon^{I+1})\\&=\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\big(\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\boldsymbol{\pi}_{(I-1)}-\boldsymbol{\pi}_{(I-1)}\big)\star_\varepsilon\boldsymbol{\pi}_{(I-1)}^\perp+\mathcal{O}_0(\varepsilon^{I+1})\\&=\big(\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\boldsymbol{\pi}_{(I-1)}-\boldsymbol{\pi}_{(I-1)}\big)\star_\varepsilon\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\boldsymbol{\pi}_{(I-1)}^\perp+\mathcal{O}_0(\varepsilon^{I+1})\\&=-\big(\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\boldsymbol{\pi}_{(I-1)}-\boldsymbol{\pi}_{(I-1)}\big)\star_\varepsilon\big(\boldsymbol{\pi}_{(I-1)}\star_\varepsilon\boldsymbol{\pi}_{(I-1)}-\boldsymbol{\pi}_{(I-1)}\big)+\mathcal{O}_0(\varepsilon^{I+1})\\&=\mathcal{O}_0(\varepsilon^{I+1})\end{aligned} \tag{6.80}$$

where we used in the last step that $\varepsilon^{2I}\boldsymbol{a}_{I-1}\star_\varepsilon\boldsymbol{a}_{I-1}$ is evidently of higher order than ε^{I+1}. As a result, the diagonal terms are determined by (6.78) while the off–diagonal contributions to $\boldsymbol{\pi}_I$ still need to be fixed. (S1–3)" provides the algebraic equations to construct them. First, the third equation in (6.76) ensures that the base clause of the induction is settled. We then assume that (S1–3)" also holds for $\boldsymbol{H}$ and $\boldsymbol{\pi}_{(I-1)}$ with the corresponding error term $\mathcal{O}_0(\varepsilon^I)$. For the iteration step,

we split again $\boldsymbol{\pi}_{(I)} = \boldsymbol{\pi}_{(I-1)} + \varepsilon^I \boldsymbol{\pi}_I$ and insert into (S1–3)", and we define a new symbol $\boldsymbol{b}_{I-1}$ such that $[\boldsymbol{\pi}_{(I-1)}, \boldsymbol{H}]_{\star_\varepsilon} =: \varepsilon^I \boldsymbol{b}_{I-1} + \mathcal{O}_0(\varepsilon^{I+1})$ where we shifted any contribution of order ε^{I+1} and higher in the Moyal commutator into the error term. This results in

$$\begin{aligned}\mathcal{O}_0(\varepsilon^{I+1}) &= \boldsymbol{H} \star_\varepsilon \boldsymbol{\pi}_{(I)} - \boldsymbol{\pi}_{(I)} \star_\varepsilon \boldsymbol{H} \\ &= \boldsymbol{H} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} - \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{H} + \varepsilon^I (\boldsymbol{H} \star_\varepsilon \boldsymbol{\pi}_I - \boldsymbol{\pi}_I \star_\varepsilon \boldsymbol{H}) \\ &= \varepsilon^I (-\boldsymbol{b}_{I-1} + \boldsymbol{H} \star_\varepsilon \boldsymbol{\pi}_I - \boldsymbol{\pi}_I \star_\varepsilon \boldsymbol{H}) \\ &= \varepsilon^I (-\boldsymbol{b}_{I-1} + [\boldsymbol{H}_0, \boldsymbol{\pi}_I]_{\mathrm{f}}). \end{aligned} \tag{6.81}$$

Consequently, the scheme requires the term in the round brackets to vanish. To extract the off–diagonal contributions of $\boldsymbol{\pi}_I$ with this relation, it is advisable to multiply it by $\boldsymbol{\pi}_0$ from the left as well as by its orthogonal complement $\boldsymbol{\pi}_0^\perp$ from the right, and to repeat the procedure with these operators exchanged. For this, we define the two off–diagonal contributions of $\boldsymbol{\pi}_I$ as $\boldsymbol{\pi}_I^{\mathrm{OD},1} := \boldsymbol{\pi}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{\pi}_0^\perp$ and $\boldsymbol{\pi}_I^{\mathrm{OD},2} := \boldsymbol{\pi}_0^\perp \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{\pi}_0$. Besides, let us denote the restriction of the zeroth order Hamilton symbol $\boldsymbol{H}_0$ which excludes the pre–selected energy band E_ν by $\boldsymbol{H}_0^\perp := \boldsymbol{H}_0 \cdot \boldsymbol{\pi}_0^\perp$. Using that $\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}_0^\perp$ commute with $\boldsymbol{H}_0$ as operators on $\mathcal{H}_{\mathrm{f}}$, this yields for the first off–diagonal part

$$\begin{aligned}\varepsilon^I \boldsymbol{\pi}_0 \cdot \boldsymbol{b}_{I-1} \cdot \boldsymbol{\pi}_0^\perp + \mathcal{O}_0(\varepsilon^{I+1}) &= \varepsilon^I (\boldsymbol{\pi}_0 \cdot \boldsymbol{H}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{\pi}_0^\perp - \boldsymbol{\pi}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{H}_0 \cdot \boldsymbol{\pi}_0^\perp) \\ &= \varepsilon^I \boldsymbol{\pi}_I^{\mathrm{OD},1} \cdot (E_\nu \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^\perp). \end{aligned} \tag{6.82}$$

By restricting to the terms of order ε^I in (6.82), this gives finally for $\boldsymbol{\pi}_I^{\mathrm{OD},1}$ and similarly for $\boldsymbol{\pi}_I^{\mathrm{OD},2}$

$$\boldsymbol{\pi}_I^{\mathrm{OD},1} = \boldsymbol{\pi}_0 \cdot \boldsymbol{b}_{I-1} \cdot (E_\nu \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^\perp)^{-1} \cdot \boldsymbol{\pi}_0^\perp, \quad \boldsymbol{\pi}_I^{\mathrm{OD},2} = -(E_\nu \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^\perp)^{-1} \cdot \boldsymbol{\pi}_0^\perp \cdot \boldsymbol{b}_{I-1} \cdot \boldsymbol{\pi}_0. \tag{6.83}$$

Again, consistency with the former derivation of $\boldsymbol{a}_{I-1}$ for the diagonal part of the Moyal projector requires to show that the diagonal part of equation (6.81) is indeed vanishing. We split this task into two steps and first derive an expression for $\boldsymbol{\pi}_0 \cdot \boldsymbol{b}_{I-1} \cdot \boldsymbol{\pi}_0$ and in a second step for $\boldsymbol{\pi}_0 \cdot [\boldsymbol{H}_0, \boldsymbol{\pi}_I]_{\mathrm{f}} \cdot \boldsymbol{\pi}_0$, namely

$$\begin{aligned}\varepsilon^I \boldsymbol{\pi}_0 \cdot \boldsymbol{b}_{I-1} \cdot \boldsymbol{\pi}_0 &= \boldsymbol{\pi}_0 \cdot (\boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{H} - \boldsymbol{H} \star_\varepsilon \boldsymbol{\pi}_{(I-1)}) \cdot \boldsymbol{\pi}_0 + \mathcal{O}_0(\varepsilon^{I+1}) \\ &= \boldsymbol{\pi}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{H} - \boldsymbol{H} \star_\varepsilon \boldsymbol{\pi}_{(I-1)}) \star_\varepsilon \boldsymbol{\pi}_{(I-1)} + \mathcal{O}_0(\varepsilon^{I+1}) \\ &= (\varepsilon^I \boldsymbol{a}_{I-1} + \boldsymbol{\pi}_{(I-1)}) \star_\varepsilon \boldsymbol{H} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} - \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{H} \star_\varepsilon (\varepsilon^I \boldsymbol{a}_{I-1} + \boldsymbol{\pi}_{(I-1)}) + \mathcal{O}_0(\varepsilon^{I+1}) \\ &= \varepsilon^I (\boldsymbol{a}_{I-1} \star_\varepsilon \boldsymbol{H} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} - \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{H} \star_\varepsilon \boldsymbol{a}_{I-1}) + \mathcal{O}_0(\varepsilon^{I+1}) \\ &= \varepsilon^I (\boldsymbol{a}_{I-1} \cdot \boldsymbol{H}_0 \cdot \boldsymbol{\pi}_0 - \boldsymbol{\pi}_0 \cdot \boldsymbol{H}_0 \cdot \boldsymbol{a}_{I-1}) + \mathcal{O}_0(\varepsilon^{I+1}) \\ &= \mathcal{O}_0(\varepsilon^{I+1}). \end{aligned} \tag{6.84}$$

Indeed, the bracket term in the last line vanishes since $\boldsymbol{H}_0 \cdot \boldsymbol{\pi}_0 = E_\nu \mathbf{1}_{\mathrm{f}}$ is proportional to the one in $\mathcal{H}_{\mathrm{f}}$ and hence commutes with $\boldsymbol{a}_{I-1}$. On the other hand, we have for $\boldsymbol{\pi}_0 \cdot [\boldsymbol{H}_0, \boldsymbol{\pi}_I]_{\mathrm{f}} \cdot \boldsymbol{\pi}_0$ that

$$\varepsilon^I \boldsymbol{\pi}_0 \cdot [\boldsymbol{H}_0, \boldsymbol{\pi}_I]_{\mathrm{f}} \cdot \boldsymbol{\pi}_0 = \varepsilon^I (\boldsymbol{\pi}_0 \cdot \boldsymbol{H}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{\pi}_0 - \boldsymbol{\pi}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{H}_0 \cdot \boldsymbol{\pi}_0) = \varepsilon^I E_\nu (\boldsymbol{\pi}_I^{\mathrm{D},1} - \boldsymbol{\pi}_I^{\mathrm{D},1}) = 0. \tag{6.85}$$

Employing the same relations, it is straightforward to derive that also

$$\varepsilon^I \boldsymbol{\pi}_0^\perp \cdot \boldsymbol{b}_{I-1} \cdot \boldsymbol{\pi}_0^\perp = \mathcal{O}_0(\varepsilon^{I+1}) \tag{6.86}$$

holds true. This proves the consistency of the relations for the off–diagonal contributions for $\boldsymbol{\pi}_I$. Collecting all terms, the final result for the coefficient of the Moyal projector at order I reads

$$\begin{aligned}\boldsymbol{\pi}_I &= \boldsymbol{\pi}_I^{\mathrm{D},0} + \boldsymbol{\pi}_I^{\mathrm{D},\perp} + \boldsymbol{\pi}_I^{\mathrm{OD},1} + \boldsymbol{\pi}_I^{\mathrm{OD},2} \\ &= -\boldsymbol{\pi}_0 \cdot \boldsymbol{a}_{I-1} \cdot \boldsymbol{\pi}_0 + \boldsymbol{\pi}_0^{\perp} \cdot \boldsymbol{a}_{I-1} \cdot \boldsymbol{\pi}_0^{\perp} + \boldsymbol{\pi}_0 \cdot \boldsymbol{b}_{I-1} \cdot (E_\nu \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^{\perp})^{-1} \cdot \boldsymbol{\pi}_0^{\perp} - (E_\nu \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^{\perp})^{-1} \cdot \boldsymbol{\pi}_0^{\perp} \cdot \boldsymbol{b}_{I-1} \cdot \boldsymbol{\pi}_0\end{aligned} \tag{6.87}$$

where $\varepsilon^I \boldsymbol{a}_{I-1} = \big(\boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} - \boldsymbol{\pi}_{(I-1)}\big)|_I$ and $\varepsilon^I \boldsymbol{b}_{I-1} = [\boldsymbol{\pi}_{(I-1)}, \boldsymbol{H}]_{\star_\varepsilon}|_I$. These relations determine $\boldsymbol{\pi}_I$ and will be used in the following applications.

6.6.2. Construction of the Moyal Unitary

The construction of the Moyal unitary follows the rules (S2)" and as before, we proceed iteratively to build $\boldsymbol{u}_{(I)}$. We assume a formal power series for the Moyal unitary up to order I, namely $\boldsymbol{u}_{(I)} = \sum_{i \leq I} \varepsilon^i \boldsymbol{u}_i$ and the symbol function $\boldsymbol{u}_0$ from (6.61) serves as the starting point for the construction scheme. Then, at zeroth order the rules (S2)" evaluate to

$$\text{(S2–1)}\, \boldsymbol{u}_0^* \cdot \boldsymbol{u}_0 - \mathbf{1}_{\mathrm{f}} = 0, \quad \text{(S2–2)}\, \boldsymbol{u}_0 \cdot \boldsymbol{u}_0^* - \mathbf{1}_{\mathrm{f}} = 0, \quad \text{(S2–3)}\, \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}_0^* - \boldsymbol{\pi}_{\mathrm{R}} = 0 \tag{6.88}$$

which are satisfied by construction of $\boldsymbol{u}_0$ and $\boldsymbol{\pi}_{\mathrm{R}}$. By induction, we assume that the rules (S2)" are satisfied for the symbol $\boldsymbol{u}_{(I-1)}$. Then, the induction assumption yields that $\boldsymbol{u}_{(I-1)}^* \star_\varepsilon \boldsymbol{u}_{(I-1)} - \mathbf{1}_{\mathrm{f}} = \mathcal{O}_0(\varepsilon^I)$, and likewise $\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{u}_{(I-1)}^* - \mathbf{1}_{\mathrm{f}} = \mathcal{O}_0(\varepsilon^I)$. To determine $\boldsymbol{u}_I$, we define the operators $\boldsymbol{c}_{I-1}$ and $\boldsymbol{d}_{I-1}$ as the contributions of order I to these equations, in particular $\boldsymbol{u}_{(I-1)}^* \star_\varepsilon \boldsymbol{u}_{(I-1)} - \mathbf{1}_{\mathrm{f}} =: \varepsilon^I \boldsymbol{c}_{I-1} + \mathcal{O}_0(\varepsilon^{I+1})$, and $\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{u}_{(I-1)}^* - \mathbf{1}_{\mathrm{f}} =: \varepsilon^I \boldsymbol{d}_{I-1} + \mathcal{O}_0(\varepsilon^{I+1})$. The corresponding equations for $\boldsymbol{u}_{(I)}$ and its adjoint $\boldsymbol{u}_{(I)}^*$ give

$$\boldsymbol{u}_{(I)}^* \star_\varepsilon \boldsymbol{u}_{(I)} - \mathbf{1}_{\mathrm{f}} = \varepsilon^I \left(\boldsymbol{c}_{I-1} + \boldsymbol{u}_I^* \cdot \boldsymbol{u}_0 + \boldsymbol{u}_0^* \cdot \boldsymbol{u}_I\right) + \mathcal{O}_0(\varepsilon^{I+1}), \tag{6.89}$$

$$\boldsymbol{u}_{(I)} \star_\varepsilon \boldsymbol{u}_{(I)}^* - \mathbf{1}_{\mathrm{f}} = \varepsilon^I \left(\boldsymbol{d}_{I-1} + \boldsymbol{u}_I \cdot \boldsymbol{u}_0^* + \boldsymbol{u}_0 \cdot \boldsymbol{u}_I^*\right) + \mathcal{O}_0(\varepsilon^{I+1}), \tag{6.90}$$

and we require that the terms in the brackets vanish. Assuming that this holds true, it is possible to extract $\boldsymbol{u}_I^*$ in both equations according to

$$\boldsymbol{u}_I^* = -(\boldsymbol{c}_{I-1} \cdot \boldsymbol{u}_0^* + \boldsymbol{u}_0^* \cdot \boldsymbol{u}_I \cdot \boldsymbol{u}_0^*) = -(\boldsymbol{u}_0^* \cdot \boldsymbol{d}_{I-1} + \boldsymbol{u}_0^* \cdot \boldsymbol{u}_I \cdot \boldsymbol{u}_0^*). \tag{6.91}$$

By comparing the two defining terms, one can relate the operators $\boldsymbol{c}_{I-1}$ and $\boldsymbol{d}_{I-1}$ by

$$\boldsymbol{c}_{I-1} = \boldsymbol{u}_0^* \cdot \boldsymbol{d}_{I-1} \cdot \boldsymbol{u}_0 \tag{6.92}$$

which is identically satisfied by the induction assumption, namely we can show that

$$\begin{aligned}\varepsilon^I(\boldsymbol{c}_{I-1} \cdot \boldsymbol{u}_0^* - \boldsymbol{u}_0^* \cdot \boldsymbol{d}_{I-1}) &= (\boldsymbol{u}_{(I-1)}^* \star_\varepsilon \boldsymbol{u}_{(I-1)} - \mathbf{1}_{\mathrm{f}}) \cdot \boldsymbol{u}_0^* - \boldsymbol{u}_0^* \cdot (\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{u}_{(I-1)}^* - \mathbf{1}_{\mathrm{f}}) + \mathcal{O}_0(\varepsilon^{I+1}) \\ &= (\boldsymbol{u}_{(I-1)}^* \star_\varepsilon \boldsymbol{u}_{(I-1)} - \mathbf{1}_{\mathrm{f}}) \star_\varepsilon \boldsymbol{u}_{(I-1)}^* - \boldsymbol{u}_{(I-1)}^* \star_\varepsilon (\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{u}_{(I-1)}^* - \mathbf{1}_{\mathrm{f}}) + \mathcal{O}_0(\varepsilon^{I+1}) \\ &= \mathcal{O}_0(\varepsilon^{I+1})\end{aligned}$$

where we used the associativity of the star product for the last manipulation. In a next step, we consider the rule (S2–3)". Since the zeroth order part of this equation is satisfied, cf. (6.88), we

assume by induction that we found $\boldsymbol{u}_{(I-1)}$ such that $\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} - \boldsymbol{\pi}_{\mathrm{R}} = \mathcal{O}_0(\varepsilon^I)$ is satisfied. We define a new operator $\boldsymbol{e}_{I-1}$ to extract the contributions of order ε^I of this equation, namely $\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} - \boldsymbol{\pi}_{\mathrm{R}} =: \varepsilon^I \boldsymbol{e}_{I-1} + \mathcal{O}_0(\varepsilon^{I+1})$. Then the induction step yields

$$\boldsymbol{u}_{(I)} \star_\varepsilon \boldsymbol{\pi}_{(I)} \star_\varepsilon \boldsymbol{u}^*_{(I)} - \boldsymbol{\pi}_{\mathrm{R}} = \varepsilon^I \left(\boldsymbol{e}_{I-1} + \boldsymbol{u}_I \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}^*_0 + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{u}^*_0 + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}^*_I \right) + \mathcal{O}_0(\varepsilon^{I+1}). \tag{6.93}$$

Consequently, we require the terms in the brackets to vanish. In this case and by means of (6.91), it holds true that

$$\begin{aligned} \boldsymbol{e}_{I-1} &= -\boldsymbol{u}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{u}^*_0 - \boldsymbol{u}_I \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}^*_0 + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot (\boldsymbol{c}_{I-1} \cdot \boldsymbol{u}^*_0 + \boldsymbol{u}^*_0 \cdot \boldsymbol{u}_I \cdot \boldsymbol{u}^*_0) && (6.94) \\ &= -\boldsymbol{u}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{u}^*_0 - \boldsymbol{u}_I \cdot \boldsymbol{u}^*_0 \cdot \boldsymbol{\pi}_{\mathrm{R}} + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{c}_{I-1} \cdot \boldsymbol{u}^*_0 + \boldsymbol{\pi}_{\mathrm{R}} \cdot \boldsymbol{u}_I \cdot \boldsymbol{u}^*_0 && (6.95) \end{aligned}$$

which transforms into an equation determining $\boldsymbol{u}_I$, namely

$$[\boldsymbol{\pi}_{\mathrm{R}}, \boldsymbol{u}_I \cdot \boldsymbol{u}^*_0]_{\mathrm{f}} = \boldsymbol{e}_{I-1} + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{u}^*_0 - \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{c}_{I-1} \cdot \boldsymbol{u}^*_0. \tag{6.96}$$

We then consider projecting this equation onto the diagonal or off–diagonal parts with respect to $\boldsymbol{\pi}_{\mathrm{R}}$ and its orthogonal complement $\boldsymbol{\pi}^\perp_{\mathrm{R}} := \mathbf{1}_{\mathrm{f}} - \boldsymbol{\pi}_{\mathrm{R}}$. As the commutator on the left hand side is anti–symmetric, this gives

$$\begin{aligned} 0 &= \boldsymbol{\pi}_{\mathrm{R}} \cdot (\boldsymbol{e}_{I-1} + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{u}^*_0 - \boldsymbol{d}_{I-1}) \cdot \boldsymbol{\pi}_{\mathrm{R}} =: \boldsymbol{R}_{ed} && (6.97) \\ &= \boldsymbol{\pi}^\perp_{\mathrm{R}} \cdot (\boldsymbol{e}_{I-1} + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{u}^*_0 - \boldsymbol{d}_{I-1}) \cdot \boldsymbol{\pi}^\perp_{\mathrm{R}} =: \boldsymbol{R}^\perp_{ed} && (6.98) \end{aligned}$$

where we introduced the symbols $\boldsymbol{R}_{ed}$ and $\boldsymbol{R}^\perp_{ed}$ for later convenience. Both equations are identically satisfied by the induction assumption. To show this, recall the result for the Moyal projector in equation (6.87) which presents the projector already as a decomposition into diagonal and off–diagonal parts. Multiplication by $\boldsymbol{u}_0$ from the left and by $\boldsymbol{u}^*_0$ from the right provides the splitting in diagonal and off–diagonal parts with respect to $\boldsymbol{\pi}_{\mathrm{R}}$ and $\boldsymbol{\pi}^\perp_{\mathrm{R}}$ such that

$$\begin{aligned} \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{u}^*_0 = &- \boldsymbol{\pi}_{\mathrm{R}} \cdot \boldsymbol{u}_0 \cdot \boldsymbol{a}_{I-1} \boldsymbol{u}^*_0 \cdot \boldsymbol{\pi}_{\mathrm{R}} + \boldsymbol{\pi}^\perp_{\mathrm{R}} \cdot \boldsymbol{u}_0 \cdot \boldsymbol{a}_{I-1} \cdot \boldsymbol{u}^*_0 \cdot \boldsymbol{\pi}^\perp_{\mathrm{R}} && (6.99) \\ &+ \boldsymbol{\pi}_{\mathrm{R}} \cdot \boldsymbol{u}_0 \cdot \boldsymbol{b}_{I-1} \cdot (E_\nu \, \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}^\perp_0)^{-1} \cdot \boldsymbol{u}^*_0 \cdot \boldsymbol{\pi}^\perp_{\mathrm{R}} - \boldsymbol{\pi}^\perp_{\mathrm{R}} \cdot \boldsymbol{u}_0 \cdot (E_\nu \, \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}^\perp_0)^{-1} \cdot \boldsymbol{b}_{I-1} \cdot \boldsymbol{u}^*_0 \cdot \boldsymbol{\pi}_{\mathrm{R}}. \end{aligned}$$

It is now obvious to restrict in equations (6.97) and (6.98) to the relevant contributions for $\boldsymbol{\pi}_I$, namely

$$\begin{aligned} \varepsilon^I \boldsymbol{R}_{ed} &= \varepsilon^I \boldsymbol{\pi}_{\mathrm{R}} \cdot (\boldsymbol{e}_{I-1} - \boldsymbol{u}_0 \cdot \boldsymbol{a}_{I-1} \cdot \boldsymbol{u}^*_0 - \boldsymbol{d}_{I-1}) \cdot \boldsymbol{\pi}_{\mathrm{R}} \\ &= \boldsymbol{\pi}_{\mathrm{R}} \cdot ((\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} - \boldsymbol{\pi}_{\mathrm{R}}) - \boldsymbol{u}_0 \cdot (\boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} - \boldsymbol{\pi}_{(I-1)}) \cdot \boldsymbol{u}^*_0) \cdot \boldsymbol{\pi}_{\mathrm{R}} \\ &\quad - \boldsymbol{\pi}_{\mathrm{R}} \cdot (\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} - \mathbf{1}_{\mathrm{f}}) \cdot \boldsymbol{\pi}_{\mathrm{R}} + \mathcal{O}_0(\varepsilon^{I+1}) \\ &= \boldsymbol{\pi}_{\mathrm{R}} \cdot (\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} - \boldsymbol{u}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} - \boldsymbol{\pi}_{(I-1)}) \star_\varepsilon \boldsymbol{u}^*_{(I-1)}) \cdot \boldsymbol{\pi}_{\mathrm{R}} \\ &\quad - \boldsymbol{\pi}_{\mathrm{R}} \cdot (\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)}) \cdot \boldsymbol{\pi}_{\mathrm{R}} + \mathcal{O}_0(\varepsilon^{I+1}) \\ &= \boldsymbol{\pi}_{\mathrm{R}} \cdot \boldsymbol{u}_{(I-1)} \star_\varepsilon (-\boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} + 2\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_{\mathrm{f}}) \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \cdot \boldsymbol{\pi}_{\mathrm{R}} + \mathcal{O}_0(\varepsilon^{I+1}) \\ &= -\boldsymbol{\pi}_{\mathrm{R}} \cdot \boldsymbol{u}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_{\mathrm{f}}) \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_{\mathrm{f}}) \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \cdot \boldsymbol{\pi}_{\mathrm{R}} + \mathcal{O}_0(\varepsilon^{I+1}). \end{aligned} \tag{6.100}$$

To show that the contributions of $\boldsymbol{R}_{ed}$ at order ε^I are indeed vanishing, we abbreviate the following $\mathcal{O}_0(\varepsilon^I)$–objects according to

$$\boldsymbol{A}_{I-1} := \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} - \boldsymbol{\pi}_{(I-1)}, \tag{6.101}$$

$$\boldsymbol{C}_{I-1} := \boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} - \mathbf{1}_\mathrm{f}, \tag{6.102}$$

$$\boldsymbol{D}_{I-1} := \boldsymbol{u}^*_{(I-1)} \star_\varepsilon \boldsymbol{u}_{(I-1)} - \mathbf{1}_\mathrm{f}, \tag{6.103}$$

$$\boldsymbol{E}_{I-1} := \boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \boldsymbol{u}^*_{(I-1)} - \boldsymbol{\pi}_\mathrm{R}. \tag{6.104}$$

With this, we continue to elaborate on $\varepsilon^I \boldsymbol{R}_{ed}$ starting from equation (6.100). In the first step, we use that $\boldsymbol{\pi}_\mathrm{R}$ does not depend on the slow phase space variables and hence the operator product of any other quantity with $\boldsymbol{\pi}_\mathrm{R}$ equals their Moyal product. Consequently, we have

$$\begin{aligned}
\varepsilon^I \boldsymbol{R}_{ed} &= -\boldsymbol{\pi}_\mathrm{R} \star_\varepsilon \boldsymbol{u}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f}) \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f}) \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_\mathrm{R} + \mathcal{O}_0(\varepsilon^{I+1}) \\
&= -(\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} - \boldsymbol{E}_{I-1}) \star_\varepsilon \boldsymbol{u}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f}) \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f}) \\
&\quad \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \star_\varepsilon (\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} - \boldsymbol{E}_{I-1}) + \mathcal{O}_0(\varepsilon^{I+1}) \\
&= -\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \star_\varepsilon \boldsymbol{u}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f})^2_{\star_\varepsilon} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \star_\varepsilon \boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \\
&\quad + \boldsymbol{E}_{I-1} \star_\varepsilon \boldsymbol{u}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f})^2_{\star_\varepsilon} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \star_\varepsilon \boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \\
&\quad + \boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \star_\varepsilon \boldsymbol{u}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f})^2_{\star_\varepsilon} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \star_\varepsilon \boldsymbol{E}_{I-1} + \mathcal{O}_0(\varepsilon^{I+1})
\end{aligned} \tag{6.105}$$

where we pushed the terms that are quadratic in $\boldsymbol{E}_{I-1}$ to the remainder $\mathcal{O}_0(\varepsilon^{I+1})$. This strategy applies for any quadratic occurence of the symbols in (6.101) – (6.104) such that the continuation of (6.105) becomes

$$\begin{aligned}
\varepsilon^I \boldsymbol{R}_{ed} &= -\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon (\boldsymbol{D}_{I-1} + \mathbf{1}_\mathrm{f}) \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f})^2_{\star_\varepsilon} \star_\varepsilon (\boldsymbol{D}_{I-1} + \mathbf{1}_\mathrm{f}) \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \\
&\quad + \boldsymbol{E}_{I-1} \star_\varepsilon \boldsymbol{u}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f})^2_{\star_\varepsilon} \star_\varepsilon (\boldsymbol{D}_{I-1} + \mathbf{1}_\mathrm{f}) \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \\
&\quad + \boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon (\boldsymbol{D}_{I-1} + \mathbf{1}_\mathrm{f}) \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f})^2_{\star_\varepsilon} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \star_\varepsilon \boldsymbol{E}_{I-1} + \mathcal{O}_0(\varepsilon^{I+1}).
\end{aligned}$$

In any of the lines, we can directly eliminate those terms that are quadratic in the operators $\boldsymbol{D}_{I-1}$ and $\boldsymbol{E}_{I-1}$. All the remaining terms admit at least one factor of the form $\boldsymbol{\pi}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f})$ or the same with factors interchanged. These factors simply evaluate to $\boldsymbol{A}_{I-1}$ and so all the contributions are at least quadratic in $\boldsymbol{A}_{I-1}, \boldsymbol{D}_{I-1}$ and $\boldsymbol{E}_{I-1}$, such that we obtain

$$\begin{aligned}
\varepsilon^I \boldsymbol{R}_{ed} &= -\boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{D}_{I-1} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f}) \star_\varepsilon \boldsymbol{A}_{I-1} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \\
&\quad - \boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{A}_{I-1} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f}) \star_\varepsilon \boldsymbol{D}_{I-1} \star_\varepsilon \boldsymbol{\pi}_{(I-1)} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \\
&\quad - \boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{A}_{I-1} \star_\varepsilon \boldsymbol{A}_{I-1} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \\
&\quad + \boldsymbol{E}_{I-1} \star_\varepsilon \boldsymbol{u}_{(I-1)} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f}) \star_\varepsilon \boldsymbol{A}_{I-1} \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \\
&\quad + \boldsymbol{u}_{(I-1)} \star_\varepsilon \boldsymbol{A}_{I-1} \star_\varepsilon (\boldsymbol{\pi}_{(I-1)} - \mathbf{1}_\mathrm{f}) \star_\varepsilon \boldsymbol{u}^*_{(I-1)} \star_\varepsilon \boldsymbol{E}_{I-1} + \mathcal{O}_0(\varepsilon^{I+1}) \\
&= \mathcal{O}_0(\varepsilon^{I+1}).
\end{aligned} \tag{6.106}$$

The very same arguments lead to the vanishing of the orthogonal part $\boldsymbol{R}^\perp_{ed}$, namely to

$$\varepsilon^I \boldsymbol{R}^\perp_{ed} = \varepsilon^I \boldsymbol{\pi}^\perp_\mathrm{R} \cdot (\boldsymbol{e}_{I-1} + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_I \cdot \boldsymbol{u}^*_0 - \boldsymbol{d}_{I-1}) \cdot \boldsymbol{\pi}^\perp_\mathrm{R} = \mathcal{O}_0(\varepsilon^{I+1}). \tag{6.107}$$

These two equations (6.106) and (6.107) consequently show that the block diagonal parts of $\boldsymbol{u}_I$ with respect to $\boldsymbol{\pi}_\mathrm{R}$ remain undetermined. Without loss of generality, we can choose them to vanish, also because $\boldsymbol{u}$ is only an auxiliary structure here. Finally, we project on the off–diagonal contributions to $\boldsymbol{u}_I$ and obtain with (6.96) and (6.99) that

$$\begin{aligned}\boldsymbol{\pi}_\mathrm{R}\cdot\boldsymbol{u}_I\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_\mathrm{R}^\perp &= \boldsymbol{\pi}_\mathrm{R}\cdot(\boldsymbol{e}_{I-1}+\boldsymbol{u}_0\cdot\boldsymbol{\pi}_I\cdot\boldsymbol{u}_0^*-\boldsymbol{d}_{I-1})\cdot\boldsymbol{\pi}_\mathrm{R}^\perp \\ &= \boldsymbol{\pi}_\mathrm{R}\cdot(\boldsymbol{e}_{I-1}+\boldsymbol{u}_0\cdot\boldsymbol{b}_{I-1}\cdot(E_\nu\,\mathbf{1}_\mathrm{f}-\boldsymbol{H}_0^\perp)^{-1}\cdot\boldsymbol{u}_0^*-\boldsymbol{d}_{I-1})\cdot\boldsymbol{\pi}_\mathrm{R}^\perp, \qquad (6.108)\\ \boldsymbol{\pi}_\mathrm{R}^\perp\cdot\boldsymbol{u}_I\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_\mathrm{R} &= -\boldsymbol{\pi}_\mathrm{R}^\perp\cdot(\boldsymbol{e}_{I-1}+\boldsymbol{u}_0\cdot\boldsymbol{\pi}_I\cdot\boldsymbol{u}_0^*-\boldsymbol{d}_{I-1})\cdot\boldsymbol{\pi}_\mathrm{R} \\ &= -\boldsymbol{\pi}_\mathrm{R}^\perp\cdot(\boldsymbol{e}_{I-1}-\boldsymbol{u}_0\cdot(E_\nu\,\mathbf{1}_\mathrm{f}-\boldsymbol{H}_0^\perp)^{-1}\cdot\boldsymbol{b}_{I-1}\cdot\boldsymbol{u}_0^*-\boldsymbol{d}_{I-1})\cdot\boldsymbol{\pi}_\mathrm{R}. \qquad (6.109)\end{aligned}$$

Eventually, the inductive equation for $\boldsymbol{u}_I$ evaluates to

$$\begin{aligned}\boldsymbol{u}_I = {}&\boldsymbol{\pi}_\mathrm{R}\cdot(\boldsymbol{e}_{I-1}+\boldsymbol{u}_0\cdot\boldsymbol{b}_{I-1}\cdot(E_\nu\,\mathbf{1}_\mathrm{f}-\boldsymbol{H}_0^\perp)^{-1}\cdot\boldsymbol{u}_0^*-\boldsymbol{d}_{I-1})\cdot\boldsymbol{\pi}_\mathrm{R}^\perp\cdot\boldsymbol{u}_0 \\ &-\boldsymbol{\pi}_\mathrm{R}^\perp\cdot(\boldsymbol{e}_{I-1}-\boldsymbol{u}_0\cdot(E_\nu\,\mathbf{1}_\mathrm{f}-\boldsymbol{H}_0^\perp)^{-1}\cdot\boldsymbol{b}_{I-1}\cdot\boldsymbol{u}_0^*-\boldsymbol{d}_{I-1})\cdot\boldsymbol{\pi}_\mathrm{R}\cdot\boldsymbol{u}_0. \qquad (6.110)\end{aligned}$$

6.6.3. Construction of the Effective Hamiltonian

The last step of the scheme consists in computing the effective Hamilton symbol $\boldsymbol{h}_\mathrm{eff}$ and in particular the effective Hamiltonian restricted to the fast subspace associated with the projector $\boldsymbol{\pi}_\mathrm{R}$ which will be denoted by $\boldsymbol{h}_{\mathrm{eff,R}}$. Recall that

$$\boldsymbol{h}_{\mathrm{eff},(I)} = \boldsymbol{u}_{(I)}\star_\varepsilon\boldsymbol{H}\star_\varepsilon\boldsymbol{u}_{(I)}^* + \mathcal{O}_0(\varepsilon^{I+1}) \qquad (6.111)$$

where we can insert $\boldsymbol{u}_{(I)}$ from the previous section. As we are mainly interested in the dynamics within the fast subspace associated with quantum number $\nu\in\mathbb{N}$, we consider the restriction

$$\boldsymbol{h}_{\mathrm{eff},(I),\mathrm{R}} = \boldsymbol{\pi}_\mathrm{R}\,\boldsymbol{u}_{(I)}\star_\varepsilon\boldsymbol{H}\star_\varepsilon\boldsymbol{u}_{(I)}^*\,\boldsymbol{\pi}_\mathrm{R} + \mathcal{O}_0(\varepsilon^{I+1}). \qquad (6.112)$$

We emphasize that the Weyl quantization $\hat{\boldsymbol{h}}_{\mathrm{eff},(I),\mathrm{R}}$ preserves the subspace $\hat{\boldsymbol{\pi}}_\mathrm{R}\mathcal{H}$. This subspace carries the orthonormal basis $\{\zeta_n\otimes\psi_\alpha\}_{n,\alpha}$ where $n\in\mathbb{N}$ is the discrete quantum number of the fast eigenstates $\zeta_n\in\mathcal{H}_\mathrm{f}$, and ψ_α denotes a (possibly generalized) orthogonal basis of $\mathcal{H}_\mathrm{s}$. As already shown before, the spectrum of $\hat{\boldsymbol{h}}_{\mathrm{eff},(I)}$ gives an approximation of order ε^{I+1} of the corresponding energy band of the original Hamiltonian $\hat{\boldsymbol{H}}$. The advantage of $\hat{\boldsymbol{h}}_{\mathrm{eff},(I)}$ is that it is effectively an operator on the rather small Hilbert space $\mathbb{C}\otimes\mathcal{H}_\mathrm{s}$ while backreaction effects between the slow and fast sector are taken care of to the given order of approximation.

This section has remained on a formal level that is valid for any perturbative order. In the following section, we derive concrete formulae in order to determine the effective Hamiltonian up to second order in the perturbations. The inductive scheme simplifies the equations significantly.

6.7. Explicit Scheme up to Second Order

This section provides all the necessary formulae that lead to the computation of the effective Hamilton symbol $\boldsymbol{h}_{\mathrm{eff},(2),\mathrm{R}}$ up to second order in the perturbations. We thereby assume that the

conditions (C1) to (C4) are all satisfied and restrict our interest to the backreaction from one single fast energy band with quantum number ν. Due to the structure of the problems that we have in mind, it is admissible to assume that the Hamilton operator admits only a zero order contribution, and we henceforth use the symbol $\boldsymbol{H}_0$ rather than $\boldsymbol{H}$. A very similar discussion of the SAPT scheme up to second order can also be found in (Schander and Thiemann 2019c) since the latter is based on our considerations here.

For the computations, it is helpful and intuitive to establish a fibre bundle perspective. The idea is to interpret for example a vector–valued function in $C^\infty(\Gamma_s, \mathcal{H}_\mathrm{f})$ as a global section of a fibre or Hilbert bundle. We assume the reader to be familiar with the standard notions of fibre bundles and refer to the works by Nakahara (2003) and Goldberg (2008). We then let $B := \Gamma_\mathrm{s} = \mathbb{R}^2$ be a smooth manifold denoted as the base space, and let $F := \mathcal{H}_\mathrm{f}$ be the fast Hilbert space denoted as the fibre space. We define the trivial Hilbert bundle $\pi : H \to B$ with $H := B \times F$ and π is the continuous bundle projection. Let $\Gamma(H)$ be the space of smooth sections $\sigma : B \to H$ of H, i.e., the space of smooth maps $\sigma(q,p)$ with $\pi \circ \sigma = id_B$. In the following, we identify points in B and F with coordinates and write $(q,p) \in B$ and $\psi \in \mathcal{H}_\mathrm{f}$. The discrete eigensolutions $\xi_n(q,p) \in \mathcal{H}_\mathrm{f}$, $n \in \mathbb{N}$, define a set of smooth sections, i.e., we can write

$$\xi_n : B \to H : (q,p) \mapsto (q,p,\xi_n(q,p)), \tag{6.113}$$

and obviously $\pi \circ \xi_n = id_B$, $\forall n \in \mathbb{N}$. Because $\boldsymbol{H}_0$ is a smooth operator–valued function on B, its discrete eigensolutions $\xi_n(q,p)$ are smooth vector–valued functions on B, and for every fixed $(q,p) \in B$ they build a complete eigenbasis of F. Their partial derivatives with respect to q and p are thus well–defined operations which yield a notion of covariant derivative from the fibre bundle perspective. To establish such a connection, let TB be the tangent bundle of the base space B, i.e., the union of the tangent spaces $T_{(q,p)}B$ which can be identified with $\mathbb{R}^2$. T^*B denotes the corresponding cotangent bundle on B, and $\Lambda(B)$ is the space of antisymmetric cotangent vectors (i.e., one–forms). We use coordinate representations to denote the elements of the tangent spaces $T_{(q,p)}B$ as $\partial_q, \partial_p \in T_{(q,p)}B$, and $\mathrm{d}q, \mathrm{d}p \in \Lambda(B)$ denote the coordinate differential one–forms. A connection of the Hilbert bundle H is a linear map

$$\nabla : \Gamma(H) \to \Gamma(H \otimes T^*B) : \sigma \mapsto \nabla(\sigma) \tag{6.114}$$

that satisfies the Leibniz rule. Here, we choose to identify the connection with the partial derivatives on B in the following way:

$$\nabla(\sigma(q,p)) := \frac{\partial \sigma}{\partial q}(q,p) \otimes \mathrm{d}q + \frac{\partial \sigma}{\partial p}(q,p) \otimes \mathrm{d}p \tag{6.115}$$

where $\sigma(q,p) \in \Gamma(H)$ is any smooth section on B. It is straightforward to show that the map is linear because the partial derivatives are linear operations. The Leibniz rule holds for any smooth function f on B and any smooth section σ, namely

$$\nabla(f\,\sigma) = f\,\nabla(\sigma) + \sigma \otimes \mathrm{d}f. \tag{6.116}$$

The definition of the connection's components requires a gauge choice, namely a specification of a basis for the fibres at each point $(q,p) \in B$. Since the zeroth order Hamilton symbol $\boldsymbol{H}_0(q,p)$

provides a complete, orthonormal basis $\{\xi_n(q,p)\}_n$ at each point (q,p) and since the bundle is trivial, it is natural to adopt this basis as our gauge choice. Any section σ may thus be decomposed as $\sigma(q,p) := \sum_n \sigma^n(q,p)\,\xi_n(q,p)$ where σ^n are the (q,p)–dependent coefficients of σ. Conventionally, we denote the connection of the basis elements ξ_n as the gauge potential $\boldsymbol{\mathcal{A}} \in C^\infty(\Lambda(B) \otimes \mathcal{L}(\mathcal{H}_\mathrm{f}))$ which is a one–form with values in the linear operators on $\mathcal{H}_\mathrm{f}$. With the gauge and coordinate choices from above, its components decompose according to

$$(\nabla\xi)_n(q,p) := (\boldsymbol{\mathcal{A}}\,\xi)_n(q,p) = \mathcal{A}_{qn}^{\ m}(q,p)\,\xi_m(q,p)\otimes \mathrm{d}q + \mathcal{A}_{pn}^{\ m}(q,p)\,\xi_m(q,p)\otimes \mathrm{d}p. \tag{6.117}$$

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

$$\frac{\partial \xi_n(q,p)}{\partial \lambda} := \mathcal{A}_{\lambda n}^{\ \ m}(q,p)\,\xi_m(q,p), \quad \lambda \in \{q,p\}. \tag{6.118}$$

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

$$\mathcal{A}_{\lambda n}^{\ \ m} = -\mathcal{A}_{\lambda m}^{\ \ n}. \tag{6.119}$$

As a consequence, the connection cannot have any diagonal contributions, namely $\mathcal{A}_{\lambda n}^{\ \ n} = 0$ for every $n \in \mathbb{N}$. These results and definitions will prove useful for the space adiabatic scheme because the Moyal product of the phase space quantization involves the derivatives of several operator–valued functions with respect to q and p, and we are going to express them in terms of the connection coefficients. Recall that the symmetric Moyal product is given at leading and subleading order for any two $\boldsymbol{f}(q,p), \boldsymbol{g}(q,p) \in C^\infty(\Gamma_\mathrm{s}, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ by

$$(\boldsymbol{f} \star_\varepsilon \boldsymbol{g})(q,p) = (\boldsymbol{f}\cdot\boldsymbol{g})(q,p) + \frac{i\varepsilon}{2}((\partial_q \boldsymbol{f})\cdot(\partial_p \boldsymbol{g}) - (\partial_p \boldsymbol{f})\cdot(\partial_q \boldsymbol{g}))(q,p) + \mathcal{O}_0(\varepsilon^2). \tag{6.120}$$

To shorten the notation, we introduce the Poisson bracket $\{\boldsymbol{f},\boldsymbol{g}\}_\mathrm{s} := (\partial_q \boldsymbol{f})\cdot(\partial_p \boldsymbol{g}) - (\partial_p \boldsymbol{f})\cdot(\partial_q \boldsymbol{g})$. The scheme then starts with the construction of the Moyal projector $\boldsymbol{\pi}$.

6.7.1. Construction of the Moyal Projector

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

$$\boldsymbol{H}_0(q,p)\,\xi_n(q,p) = E_n(q,p)\,\xi_n(q,p), \quad \xi_n(q,p) \in \mathcal{H}_\mathrm{f}. \tag{6.121}$$

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

$$\boldsymbol{\pi}_0(q,p) := \xi_\nu(q,p)\,\langle \xi_\nu(q,p), \cdot \rangle_\mathrm{f}. \tag{6.122}$$

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

$$\text{(S1–1)}\ \boldsymbol{\pi}\cdot\boldsymbol{\pi}_0 - \boldsymbol{\pi}_0 = 0, \quad \text{(S1–2)}\ \boldsymbol{\pi}_0^* = \boldsymbol{\pi}_0, \quad \text{(S1–3)}\ [\boldsymbol{\pi}_0, \boldsymbol{H}_0] = 0, \tag{6.123}$$

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

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

By means of the series expansion of $\boldsymbol{\pi}_{(1)}$ and the star product in equation (6.120), the expansion of the first condition (S1–1) in ε yields up to first order

$$\boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_0 + \varepsilon\left(\frac{i}{2}\{\boldsymbol{\pi}_0,\boldsymbol{\pi}_0\}_\mathrm{s} + \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1 + \boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0\right) = \boldsymbol{\pi}_0 + \varepsilon\,\boldsymbol{\pi}_1 + \mathcal{O}_0(\varepsilon^2). \tag{6.124}$$

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

$$0 \overset{!}{=} \boldsymbol{a}_1 + \boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_0 + \boldsymbol{\pi}_0\cdot\boldsymbol{\pi}_1 - \boldsymbol{\pi}_1 \quad \text{with} \quad \boldsymbol{a}_1 := \frac{i}{2}\{\boldsymbol{\pi}_0,\boldsymbol{\pi}_0\}_\mathrm{s} \tag{6.125}$$

where we tie in with the notation of the general construction scheme in the previous section. The evaluation of the symbol $\boldsymbol{a}_1$ requires to build the q– and p–derivatives of $\boldsymbol{\pi}_0(q,p)$. Using the connection components $\mathcal{A}_{\lambda n}{}^{m}(q,p)$ from above and the functional representation of $\boldsymbol{\pi}_0$ due to Riesz in equation (6.122), we obtain

$$\frac{\partial\boldsymbol{\pi}_0}{\partial\lambda} = \mathcal{A}_{\lambda\nu}{}^{m}(\xi_\nu\langle\xi_m,\cdot\rangle_\mathrm{f} + \xi_m\langle\xi_\nu,\cdot\rangle_\mathrm{f}), \tag{6.126}$$

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

$$\boldsymbol{a}_1 = \frac{i}{2}\left[\frac{\partial\boldsymbol{\pi}_0}{\partial q}, \frac{\partial\boldsymbol{\pi}_0}{\partial p}\right]_\mathrm{f} = \mathcal{A}_{q\nu}{}^{m}\,\mathcal{A}_{p\nu}{}^{k}\,(\xi_m\,\langle\xi_k,\cdot\rangle_\mathrm{f} - \xi_k\,\langle\xi_m,\cdot\rangle_\mathrm{f})\,. \tag{6.127}$$

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

$$\boldsymbol{\pi}_1^\mathrm{D} = -\boldsymbol{\pi}_0\cdot\boldsymbol{a}_1\cdot\boldsymbol{\pi}_0 + \boldsymbol{\pi}_0^\perp\cdot\boldsymbol{a}_1\cdot\boldsymbol{\pi}_0^\perp = \boldsymbol{\pi}_0^\perp\cdot\boldsymbol{a}_1\cdot\boldsymbol{\pi}_0^\perp \tag{6.128}$$

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

Condition (S1–3): $\boldsymbol{H} \star_\varepsilon \boldsymbol{\pi} - \boldsymbol{\pi} \star_\varepsilon \boldsymbol{H} = 0$

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

$$[\boldsymbol{H}_0, \boldsymbol{\pi}_0]_{\mathrm{f}} + \varepsilon \left(\frac{i}{2} \{\boldsymbol{H}_0, \boldsymbol{\pi}_0\}_{\mathrm{s}} - \frac{i}{2} \{\boldsymbol{\pi}_0, \boldsymbol{H}_0\}_{\mathrm{s}} + \boldsymbol{H}_0 \cdot \boldsymbol{\pi}_1 - \boldsymbol{\pi}_1 \cdot \boldsymbol{H}_0 \right) = \mathcal{O}_0(\varepsilon^2). \tag{6.129}$$

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

$$0 \stackrel{!}{=} -\boldsymbol{b}_1 + [\boldsymbol{H}_0, \boldsymbol{\pi}_1]_{\mathrm{f}} \quad \text{with} \quad \boldsymbol{b}_1 := \frac{i}{2} \left(\{\boldsymbol{H}_0, \boldsymbol{\pi}_0\}_{\mathrm{s}} - \{\boldsymbol{\pi}_0, \boldsymbol{H}_0\}_{\mathrm{s}} \right). \tag{6.130}$$

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

$$\begin{aligned} \boldsymbol{\pi}_1^{\mathrm{OD}} &= \boldsymbol{\pi}_0 \cdot \boldsymbol{b}_1 \cdot \boldsymbol{\pi}_0^\perp \cdot (E_\nu \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^\perp)^{-1} - (E_\nu \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^\perp)^{-1} \cdot \boldsymbol{\pi}_0^\perp \cdot \boldsymbol{b}_1 \cdot \boldsymbol{\pi}_0 \\ &= \frac{i}{2} \big[\boldsymbol{\pi}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}} \cdot (E_\nu \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^\perp)^{-1} \cdot \boldsymbol{\pi}_0^\perp + (E_\nu \mathbf{1}_{\mathrm{f}} - \boldsymbol{H}_0^\perp)^{-1} \cdot \boldsymbol{\pi}_0^\perp \cdot \{\boldsymbol{H}_0 + E_\nu \mathbf{1}_{\mathrm{f}}, \boldsymbol{\pi}_0\}_{\mathrm{s}} \cdot \boldsymbol{\pi}_0 \big]. \end{aligned} \tag{6.131}$$

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

$$\boldsymbol{H}_0(q,p) = \sum_{n \in \mathbb{N}} E_n(q,p)\, \xi_n(q,p) \langle \xi_n(q,p), \cdot \rangle_{\mathrm{f}} \tag{6.132}$$

where $E_n(q,p)$ is the real–valued energy band function for the quantum number n. Consequently, derivations of $\boldsymbol{H}_0(q,p)$ with respect to q and p consist of three contributions for every n due to the product rule. This is for example relevant for the Poisson brackets that enter equation (6.131). To illustrate the explicit evaluation of the respective terms, we compute the left contributions of the first term in $\boldsymbol{\pi}_1^{\mathrm{OD}}$, i.e.,

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

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

$$\boldsymbol{\pi}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{H}_0 + E_\nu \mathbf{1}_\mathrm{f}\}_\mathrm{s} =: \sum_n \xi_\nu \langle \xi_n, \cdot \rangle_\mathrm{f} A_{\nu n}(q,p) \tag{6.133}$$

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

$$A_{\nu n} := \left[\left[\mathcal{A}_{q\nu}{}^n \frac{\partial(E_n + E_\nu)}{\partial p} - \mathcal{A}_{p\nu}{}^n \frac{\partial(E_n + E_\nu)}{\partial q}\right] + (E_n - E_m)\left(\mathcal{A}_{p\nu}{}^m \mathcal{A}_{qm}{}^n - \mathcal{A}_{q\nu}{}^m \mathcal{A}_{pm}{}^n\right)\right]. \tag{6.134}$$

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

$$\begin{aligned} &\frac{i}{2}\boldsymbol{\pi}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{H}_0 + E_\nu \mathbf{1}_\mathrm{f}\}_\mathrm{s} \cdot (E_\nu \mathbf{1}_\mathrm{f} - \boldsymbol{H}_0^\perp)^{-1} \cdot \boldsymbol{\pi}_0^\perp \\ &\quad = \frac{i}{2}\sum_n \xi_\nu \langle \xi_n, \cdot \rangle_\mathrm{f} A_{\nu n}(q,p) \cdot \sum_{l \neq \nu} \frac{\xi_l \langle \xi_l, \cdot \rangle_\mathrm{f}}{E_\nu - E_l} = \frac{i}{2}\sum_{n \neq \nu} \frac{A_{\nu n}}{E_\nu - E_n}\, \xi_\nu \langle \xi_n, \cdot \rangle_\mathrm{f}. \end{aligned} \tag{6.135}$$

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

$$\boldsymbol{\pi}_1^{\mathrm{OD}} = \frac{i}{2}\sum_{n \neq \nu} \frac{A_{\nu n}}{E_\nu - E_n} \left(\xi_\nu \langle \xi_n, \cdot \rangle_\mathrm{f} - \xi_n \langle \xi_\nu, \cdot \rangle_\mathrm{f}\right). \tag{6.136}$$

Thereby, note that any of the functions $A_{\nu n}$, E_n and ξ_n are real–valued. It is easy to check that indeed, an explicit evaluation of the second summand in equation (6.131) for $\boldsymbol{\pi}_1^{\mathrm{OD}}$ yields the same result. We have thus determined all contributions to $\boldsymbol{\pi}_{(1)}$. The abstract results that we provide here will be illustrated in simple toy model examples in the following sections, and we will see that many of the terms simplify significantly. For closing this section, we emphasize that $\boldsymbol{\pi}_{(1)}(q,p)$ depends on the heavy phase space variables. Quantizing it with respect to the slow phase space variables yields a non–trivial operator with respect to the heavy subsystem and hence, does not simplify the task to find (approximate) solutions for the quantum problem. The next step of the scheme consists in constructing a unitary symbol $\boldsymbol{u}$ which maps the dynamical subspace related to $\boldsymbol{\pi}_{(1)}$ to a suitable reference subspace $\mathcal{K}_\mathrm{f} \subset \mathcal{H}_\mathrm{f}$.

6.7.2. Construction of the Moyal Unitary

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

$$\boldsymbol{\pi}_\mathrm{R} := \xi_\nu(q_0,p_0) \left\langle \xi_\nu(q_0,p_0), \cdot \right\rangle_\mathrm{f} =: \zeta_\nu \langle \zeta_\nu, \cdot \rangle_\mathrm{f}. \tag{6.137}$$

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

$$\boldsymbol{u}_0(q,p) := \sum_{n\geq 0} \zeta_n \left\langle \xi_n(q,p), \cdot \right\rangle_\mathrm{f} \tag{6.138}$$

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

$$\text{(S2–1)}\,\boldsymbol{u}_0 \cdot \boldsymbol{u}_0^* = \mathbf{1}_\mathrm{f}, \quad \text{(S2–2)}\,\boldsymbol{u}_0^* \cdot \boldsymbol{u}_0 = \mathbf{1}_\mathrm{f}, \quad \text{(S2–3)}\,\boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}_0^* = \boldsymbol{\pi}_\mathrm{R}. \tag{6.139}$$

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

Conditions (S2–1) and (S2–2): $\boldsymbol{u} \star_\varepsilon \boldsymbol{u}^* = \mathbf{1}_f = \boldsymbol{u}^* \star_\varepsilon \boldsymbol{u}$

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

$$\boldsymbol{u}_0 \cdot \boldsymbol{u}_0^* - \mathbf{1}_\mathrm{f} + \varepsilon \left(\frac{i}{2}\{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_\mathrm{s} + 2\,\boldsymbol{h}_1 \right) = \mathcal{O}_0(\varepsilon^2), \tag{6.140}$$

and likewise for the second condition (S2–2). At zeroth order, the resulting conditions $\boldsymbol{u}_0 \cdot \boldsymbol{u}_0^* - \mathbf{1}_\mathrm{f} = 0$, and $\boldsymbol{u}_0^* \cdot \boldsymbol{u}_0 - \mathbf{1}_\mathrm{f} = 0$ are trivially satisfied for the choice of $\boldsymbol{u}_0$ in (6.206). For the first order contribution, the scheme requires that the terms in the brackets vanish identically. This yields a determining equation for $\boldsymbol{h}_1$ for which we evaluate

$$\frac{\partial \boldsymbol{u}_0}{\partial \lambda} = \sum_n \zeta_n \left\langle \frac{\partial \xi_n}{\partial \lambda}, \cdot \right\rangle_\mathrm{f} = \sum_n \mathcal{A}_{\lambda n}{}^m \zeta_n \left\langle \xi_m, \right\rangle_\mathrm{f}, \tag{6.141}$$

$$\frac{\partial \boldsymbol{u}_0^*}{\partial \lambda} = \sum_n \frac{\partial \xi_n}{\partial \lambda} \langle \zeta_n, \cdot \rangle_\mathrm{f} = \sum_n \mathcal{A}_{\lambda n}{}^m\, \xi_m \langle \zeta_n, \cdot \rangle_\mathrm{f}. \tag{6.142}$$

The total hermitian part $\boldsymbol{u}_1^\mathrm{h} := \boldsymbol{h}_1 \cdot \boldsymbol{u}_0$ is then given according to equation (6.207) by

$$\boldsymbol{u}_1^\mathrm{h} = -\frac{i}{4}\{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_\mathrm{s} \cdot \boldsymbol{u}_0 = \frac{i}{4} \sum_{n,m,k} \left(\mathcal{A}_{qn}{}^m \mathcal{A}_{pm}{}^k - \mathcal{A}_{pn}{}^m \mathcal{A}_{qm}{}^k \right) \zeta_n \langle \xi_k, \cdot \rangle_\mathrm{f}. \tag{6.143}$$

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

Condition (S2–3): $\boldsymbol{u} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{u}^* = \boldsymbol{\pi}_R$

We evaluate condition (S2–3) up to first order in the perturbations and obtain at zeroth order the obvious result $\boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}_0^* = \boldsymbol{\pi}_\mathrm{R}$. In order to determine the first order contributions and hence $\boldsymbol{k}_1$,

we closely follow Teufel (2003, p. 86) and make the following definition:

$$\boldsymbol{w}_{(1)} := \boldsymbol{u}_0 + \varepsilon \boldsymbol{h}_1 \cdot \boldsymbol{u}_0 = \boldsymbol{u}_{(1)} - \varepsilon \boldsymbol{k}_1 \cdot \boldsymbol{u}_0 \tag{6.144}$$

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

$$\boldsymbol{w}_{(1)} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{w}^*_{(1)} - \boldsymbol{\pi}_\mathrm{R} =: \varepsilon \boldsymbol{K}_1 + \mathcal{O}_0(\varepsilon^2). \tag{6.145}$$

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

$$\boldsymbol{u}_{(1)} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{u}^*_{(1)} - \boldsymbol{\pi}_\mathrm{R} =: \varepsilon \left(\boldsymbol{K}_1 + [\boldsymbol{k}_1, \boldsymbol{\pi}_\mathrm{R}]_\mathrm{f} \right) + \mathcal{O}_0(\varepsilon^2). \tag{6.146}$$

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

$$\boldsymbol{\pi}_\mathrm{R} \cdot \boldsymbol{K}_1 \cdot \boldsymbol{\pi}_\mathrm{R} = 0 = \boldsymbol{\pi}^\perp_\mathrm{R} \cdot \boldsymbol{K}_1 \cdot \boldsymbol{\pi}^\perp_\mathrm{R}. \tag{6.147}$$

To show the second equality, we use that $\boldsymbol{w}_{(1)}$ satisfies (S1–1) and (S1–2) up to second order in the perturbations such that $\boldsymbol{\pi}^\perp_0$ can be written as

$$\begin{aligned} \mathbf{1}_\mathrm{f} - \boldsymbol{\pi}_\mathrm{R} &= \boldsymbol{w}_{(1)} \star_\varepsilon \boldsymbol{w}^*_{(1)} - \boldsymbol{\pi}_\mathrm{R} + \mathcal{O}_0(\varepsilon^2) = \boldsymbol{w}_{(1)} \star_\varepsilon \boldsymbol{w}^*_{(1)} + \boldsymbol{w}_{(1)} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{w}^*_{(1)} + \varepsilon \boldsymbol{K}_1 + \mathcal{O}_0(\varepsilon^2) \\ &= \boldsymbol{w}_{(1)} \star_\varepsilon (\mathbf{1}_\mathrm{f} - \boldsymbol{\pi}) \star_\varepsilon \boldsymbol{w}^*_{(1)} + \varepsilon \boldsymbol{K}_1 + \mathcal{O}_0(\varepsilon^2). \end{aligned} \tag{6.148}$$

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

$$\begin{aligned} \boldsymbol{\pi}^\perp_\mathrm{R} \cdot \boldsymbol{K}_1 \cdot \boldsymbol{\pi}^\perp_\mathrm{R} &= \left[\frac{1}{\varepsilon} \boldsymbol{\pi}^\perp_\mathrm{R} \cdot (\boldsymbol{w}_{(1)} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{w}^*_{(1)} - \boldsymbol{\pi}_\mathrm{R}) \cdot \boldsymbol{\pi}^\perp_\mathrm{R} \right]_0 = \left[\frac{1}{\varepsilon} \boldsymbol{\pi}^\perp_\mathrm{R} \star_\varepsilon \boldsymbol{w}_{(1)} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{w}^*_{(1)} \star_\varepsilon \boldsymbol{\pi}^\perp_\mathrm{R} \right]_0 \\ &= \left[\frac{1}{\varepsilon} \boldsymbol{\pi}^\perp_\mathrm{R} \star_\varepsilon \boldsymbol{w}_{(1)} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{w}^*_{(1)} \star_\varepsilon (\boldsymbol{w}_{(1)} \star_\varepsilon (\mathbf{1}_\mathrm{f} - \boldsymbol{\pi}) \star_\varepsilon \boldsymbol{w}^*_{(1)} + \varepsilon \boldsymbol{K}_1) \right]_0 \\ &= \left[(\boldsymbol{w}_{(1)} \star_\varepsilon (\mathbf{1}_\mathrm{f} - \boldsymbol{\pi}) \star_\varepsilon \boldsymbol{w}^*_{(1)} + \varepsilon \boldsymbol{K}_1) \star_\varepsilon \boldsymbol{w}_{(1)} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{w}^*_{(1)} \star_\varepsilon \boldsymbol{K}_1 \right]_0 \\ &= 0. \end{aligned} \tag{6.149}$$

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

$$\boldsymbol{K}_1 = \boldsymbol{h}_1 \cdot \boldsymbol{\pi}_\mathrm{R} + \boldsymbol{\pi}_\mathrm{R} \cdot \boldsymbol{h}_1 + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1 \cdot \boldsymbol{u}^*_0 + \frac{i}{2} \boldsymbol{u}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{u}^*_0\}_\mathrm{s} + \frac{i}{2} \{\boldsymbol{u}_0, \boldsymbol{u}^*_0\}_\mathrm{s} \cdot \boldsymbol{\pi}_\mathrm{R}. \tag{6.150}$$

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

$$\left[\boldsymbol{\pi}_{\mathrm{R}}, \boldsymbol{u}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{u}_0^*\}_{\mathrm{s}}\right]_{\mathrm{f}} = \left[\boldsymbol{\pi}_{\mathrm{R}}, \{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_{\mathrm{s}}\right]_{\mathrm{f}} \tag{6.151}$$

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

$$\boldsymbol{u}_1^{\mathrm{ah}} = \left[\boldsymbol{\pi}_{\mathrm{R}}, \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1^{\mathrm{OD}} \cdot \boldsymbol{u}_0^*\right]_{\mathrm{f}} \cdot \boldsymbol{u}_0 + \frac{i}{4}\left[\boldsymbol{\pi}_{\mathrm{R}}, \{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_{\mathrm{s}}\right]_{\mathrm{f}} \cdot \boldsymbol{u}_0. \tag{6.152}$$

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

6.7.3. Construction of the Effective Hamiltonian

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

$$\boldsymbol{h}_{\mathrm{eff},0,\mathrm{R}} = \boldsymbol{\pi}_{\mathrm{R}} \cdot \boldsymbol{u}_0 \cdot \boldsymbol{H}_0 \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\mathrm{R}} = \sum_n E_n(q,p)\, \zeta_n \langle \zeta_n, \cdot \rangle_{\mathrm{f}}. \tag{6.153}$$

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

$$\boldsymbol{u} \star_\varepsilon \boldsymbol{H} - \boldsymbol{h}_{\mathrm{eff},0} \star_\varepsilon \boldsymbol{u} = \varepsilon\, \boldsymbol{h}_{\mathrm{eff},1} \star_\varepsilon \boldsymbol{u} + \mathcal{O}_0(\varepsilon^2) = \varepsilon\, \boldsymbol{h}_{\mathrm{eff},1} \cdot \boldsymbol{u}_0 + \mathcal{O}_0(\varepsilon^2). \tag{6.154}$$

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

$$\boldsymbol{h}_{\mathrm{eff},1} = \left[\boldsymbol{u}_1 \cdot \boldsymbol{H}_0 - \boldsymbol{h}_{\mathrm{eff},0} \cdot \boldsymbol{u}_1 + \frac{i}{2}\{\boldsymbol{u}_0, \boldsymbol{H}_0\}_{\mathrm{s}} - \frac{i}{2}\{\boldsymbol{h}_{\mathrm{eff},0}, \boldsymbol{u}_0\}_{\mathrm{s}}\right] \cdot \boldsymbol{u}_0^*. \tag{6.155}$$

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

$$\begin{aligned} \boldsymbol{h}_{\mathrm{eff},1,\mathrm{R}} &= \boldsymbol{\pi}_{\mathrm{R}} \cdot \boldsymbol{h}_{\mathrm{eff},1} \cdot \boldsymbol{\pi}_{\mathrm{R}} = \boldsymbol{\pi}_{\mathrm{R}} \cdot \boldsymbol{u}_1 \cdot (\boldsymbol{H}_0 - E_\nu) \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\mathrm{R}} + \frac{i}{2}\, \boldsymbol{\pi}_{\mathrm{R}} \cdot \{\boldsymbol{u}_0, \boldsymbol{H}_0 + E_\nu\, \mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\mathrm{R}} \\ &= \frac{i}{2}\, \boldsymbol{\pi}_{\mathrm{R}} \cdot \{\boldsymbol{u}_0, \boldsymbol{H}_0 + E_\nu\, \mathbf{1}_{\mathrm{f}}\}_{\mathrm{s}} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\mathrm{R}} \end{aligned} \tag{6.156}$$

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

$$\boldsymbol{\pi}_{\mathrm{R}} \cdot \frac{\partial \boldsymbol{u}_0}{\partial \lambda} = \mathcal{A}_{\lambda\nu}{}^m\, \zeta_\nu \langle \xi_m, \cdot \rangle_{\mathrm{f}} = \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \frac{\partial \boldsymbol{\pi}_0}{\partial \lambda}. \tag{6.157}$$

As a consequence, we can reformulate $\boldsymbol{h}_{\text{eff,1,R}}$ such that it is possible to use the identities that we found for determining $\boldsymbol{\pi}_1^{\text{OD}}$, in particular (6.133) and the subsequent definition. This gives

$$\begin{aligned}\boldsymbol{h}_{\text{eff,1,R}} &= \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\text{R}} = \sum_n \zeta_\nu \langle \xi_n, \cdot \rangle_{\text{f}} A_{\nu n} \, \xi_\nu \langle \zeta_\nu, \cdot \rangle_{\text{f}} \\ &= A_{\nu\nu} \, \zeta_\nu \langle \zeta_\nu, \cdot \rangle_{\text{f}} = 0. \end{aligned} \tag{6.158}$$

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

$$\begin{aligned}\boldsymbol{h}_{\text{eff,2,R}} = \boldsymbol{\pi}_{\text{R}} \cdot \Big[&-\boldsymbol{h}_{\text{eff,1}} \cdot \boldsymbol{u}_1 + \frac{i}{2}\{\boldsymbol{u}_1, \boldsymbol{H}_0\}_{\text{s}} - \frac{i}{2}\{E_\nu, \boldsymbol{u}_1\}_{\text{s}} - \frac{i}{2}\{\boldsymbol{h}_{\text{eff,1}}, \boldsymbol{u}_0\}_{\text{s}} + [\, \boldsymbol{u}_0 \star_\varepsilon \boldsymbol{H}_0]_2 \\ &- [E_\nu \star_\varepsilon \boldsymbol{u}_0]_2 \Big] \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\text{R}} \end{aligned} \tag{6.159}$$

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

$$\begin{aligned}\boldsymbol{\pi}_{\text{R}} \cdot \boldsymbol{h}_{\text{eff,1,R}} &= \boldsymbol{\pi}_{\text{R}} \cdot \boldsymbol{u}_1 \cdot (\boldsymbol{H}_0 - E_\nu \mathbf{1}_{\text{f}}) \cdot \boldsymbol{u}_0^* + \frac{i}{2} \boldsymbol{\pi}_{\text{R}} \cdot \{\boldsymbol{u}_0, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot \boldsymbol{u}_0 \\ &= -\frac{i}{2} \boldsymbol{\pi}_{\text{R}} \cdot \boldsymbol{u}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot (\mathbf{1}_{\text{f}} - \boldsymbol{\pi}_0) \cdot \boldsymbol{u}_0^* + \frac{i}{2} \boldsymbol{\pi}_{\text{R}} \cdot \{\boldsymbol{u}_0, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot \boldsymbol{u}_0^* \\ &\quad - \frac{i}{4} \boldsymbol{\pi}_{\text{R}} \cdot \big[\{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_{\text{s}} - \boldsymbol{\pi}_{\text{R}} \cdot \{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_{\text{s}} + \{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_{\text{s}} \cdot \boldsymbol{\pi}_{\text{R}}\big] \cdot \boldsymbol{u}_0 \cdot (\boldsymbol{H}_0 - E_\nu \mathbf{1}_{\text{f}}) \cdot \boldsymbol{u}_0^* \\ &= \frac{i}{2} \boldsymbol{\pi}_{\text{R}} \cdot \{\boldsymbol{u}_0, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}_0^* = 0. \end{aligned} \tag{6.160}$$

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

$$\begin{aligned}&\frac{i}{2} \{\boldsymbol{\pi}_{\text{R}} \cdot \boldsymbol{u}_1, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\text{R}} \\ &\quad = \frac{1}{4} \{\{\boldsymbol{\pi}_{\text{R}} \cdot \boldsymbol{u}_0, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot (\boldsymbol{H}_0 - E_\nu \mathbf{1}_{\text{f}})^{-1} \cdot \boldsymbol{\pi}_0^\perp, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\text{R}}. \end{aligned} \tag{6.161}$$

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

$$\begin{aligned}&\frac{i}{2} \{\boldsymbol{\pi}_{\text{R}} \cdot \boldsymbol{u}_1, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\text{R}} \\ &= -\frac{1}{4} \sum_{n \neq \nu} \left[\frac{\partial}{\partial q} \left[\frac{A_{\nu n}}{E_\nu - E_n} \right] (E_\nu - E_n) \mathcal{A}_{p\nu}^{\ n} - 2 \frac{\partial E_\nu}{\partial p} \frac{A_{\nu n} \mathcal{A}_{q\nu}^{\ n}}{E_\nu - E_n} - A_{\nu n} \mathcal{A}_{qn}^{\ m} \mathcal{A}_{pm}^{\ \nu} \frac{E_\nu - E_m}{E_\nu - E_n} \right] \\ &\quad + \frac{1}{4} \sum_{n \neq \nu} \Big[\qquad --- \qquad (p \leftrightarrow q) \qquad --- \qquad \Big] \end{aligned} \tag{6.162}$$

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

$$\begin{aligned} &\boldsymbol{\pi}_\text{R} \cdot \Big[[\boldsymbol{u}_0 \star_\varepsilon \boldsymbol{H}_0]_2 - [E_\nu \star_\varepsilon \boldsymbol{u}_0]_2 \Big] \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_\text{R} \\ &= \boldsymbol{\pi}_\text{R} \cdot \left[-\frac{1}{8} \frac{\partial^2 \boldsymbol{u}_0}{\partial q^2} \frac{\partial^2 (\boldsymbol{H}_0 - E_\nu)}{\partial p^2} + \frac{1}{4} \frac{\partial^2 \boldsymbol{u}_0}{\partial p \, \partial q} \frac{\partial^2 (\boldsymbol{H}_0 - E_\nu)}{\partial q \, \partial p} - \frac{1}{8} \frac{\partial^2 \boldsymbol{u}_0}{\partial p^2} \frac{\partial^2 (\boldsymbol{H}_0 - E_\nu)}{\partial q^2} \right] \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_\text{R}. \end{aligned} \tag{6.163}$$

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

$$\boldsymbol{\pi}_\text{R} \cdot \left[-\frac{1}{8} \frac{\partial^2 \boldsymbol{u}_0}{\partial q^2} \frac{\partial^2 (\boldsymbol{H}_0 - E_\nu)}{\partial p^2} \right] \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_\text{R} =: \; B_{\text{eff},1}(q,p) \, \boldsymbol{\pi}_\text{R} \tag{6.164}$$

$$\boldsymbol{\pi}_\text{R} \cdot \left[\frac{1}{4} \frac{\partial^2 \boldsymbol{u}_0}{\partial p \, \partial q} \frac{\partial^2 (\boldsymbol{H}_0 - E_\nu)}{\partial q \, \partial p} \right] \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_\text{R} \; =: \; B_{\text{eff},2}(q,p) \, \boldsymbol{\pi}_\text{R}, \tag{6.165}$$

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

$$\begin{aligned} B_{\text{eff},1}(q,p) = -\frac{1}{8} \Bigg[& 2 \, \frac{\partial (E_n - E_\nu)}{\partial p} \mathcal{A}_{pn}{}^{\nu} + (E_n - E_\nu) \frac{\partial \mathcal{A}_{pn}{}^{\nu}}{\partial p} + (E_n - 2E_m + E_\nu) \mathcal{A}_{pn}{}^{m} \mathcal{A}_{pm}{}^{\nu} \Bigg] \\ & \cdot \left[\frac{\partial \mathcal{A}_{q\nu}{}^{n}}{\partial q} + \mathcal{A}_{q\nu}{}^{k} \mathcal{A}_{qk}{}^{n} \right] \cdot \boldsymbol{\pi}_\text{R}, \\ B_{\text{eff},2}(q,p) = \frac{1}{4} \Bigg[& \frac{\partial (E_n - E_\nu)}{\partial q} \mathcal{A}_{p\nu}{}^{n} + \frac{\partial (E_n - E_\nu)}{\partial p} \mathcal{A}_{q\nu}{}^{n} + (E_n - E_\nu) \frac{\partial \mathcal{A}_{q\nu}{}^{n}}{\partial p} \\ & + (E_m - E_\nu) \mathcal{A}_{q\nu}{}^{m} \mathcal{A}_{pm}{}^{n} + (E_m - E_n) \mathcal{A}_{p\nu}{}^{m} \mathcal{A}_{qm}{}^{n} \Bigg] \left[\frac{\partial \mathcal{A}_{qn}{}^{\nu}}{\partial p} - \mathcal{A}_{pn}{}^{k} \mathcal{A}_{qk}{}^{\nu} \right]. \end{aligned} \tag{6.166}$$

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

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

and we emphasize that the last term simply arises from the first term by interchanging any occurence of q by p and vice versa. These contributions together with those in equation (6.162) build then the total effective Hamiltonian symbol $\boldsymbol{h}_{\text{eff},2,\text{R}}(q,p)$. However lengthy these expressions might be, in the application to the models that we consider here, most of the terms vanish or enter at higher orders in the perturbative ε–scheme. To illustrate this, we consider a simple toy model consisting of two coupled oscillators.

6.8. An Example: Coupled Oscillators

This section applies the space adiabatic perturbation scheme to a simple oscillator toy model, and it is based and largely taken from (Neuser, Schander, and Thiemann 2019). More precisely, the quantum system comprises two coupled subsystems: An anharmonic oscillator which can be identified with a heavy mass $M \in \mathbb{R}^+$, and a harmonic oscillator associated with a lighter mass $m \in \mathbb{R}^+$. We require the mass ratio $\varepsilon^2 := \frac{m}{M}$ to be small. Accordingly, the anharmonic oscillator with mass M admits a much smaller rate of change than the harmonic oscillator with mass m. In the following, we refer to the heavy anharmonic subsystem with phase space variables $(q, P) \in \Gamma_\mathrm{s} = \mathbb{R}^2$, while for the light harmonic oscillator, we introduce the phase space variables $(x, y) \in \Gamma_\mathrm{f} = \mathbb{R}^2$. The classical Hamiltonian associated with the model is given as the four–times differentiable function on the cartesian product of phase spaces $\Gamma_\mathrm{s} \times \Gamma_\mathrm{f}$

$$H(q, P, x, y) = \frac{P^2}{2M} + \frac{y^2}{2m} + \frac{1}{2} m\, \omega(q)^2 \cdot x^2 \quad \in C^4(\Gamma_\mathrm{s} \times \Gamma_\mathrm{f}, \mathbb{R}) \tag{6.167}$$

where we have introduced the function

$$\omega(q) := \omega_0 \left(1 + \frac{q^2}{L^2}\right) \quad \in C^2(\Gamma_\mathrm{s}, \mathbb{R}^+). \tag{6.168}$$

The function ω mediates the coupling between the two oscillators and can be understood as a q–dependent frequency of the light harmonic oscillator. The parameter $L \in \mathbb{R}^+$ has the dimension of a length and plays the role of a coupling constant of the subsystems. The coupling vanishes in the limit $L \to \infty$. We quantize the system and start by considering the light harmonic oscillator. We specify the state space as a standard L^2–space and denote it as $L^2(\mathbb{R}, \mathrm{d}x)$. The quantum operators of the canonical variables x and y will be indicated as bold letters and shall act on the vectors in $L^2(\mathbb{R})$ in the known way as multiplication and derivative operators. In the following, we set $\hbar \equiv 1$. Position and momentum operator of the light oscillator satisfy the formal commutation relation

$$[\boldsymbol{x}, \boldsymbol{y}]_\mathrm{f} = i\, \mathbf{1}_\mathrm{f}. \tag{6.169}$$

Since the classical Hamilton function $H(q, P, x, y)$ does not contain any mixed products of the canonical variables x and y, there is no ordering choice to be made for the quantum theory. For the heavy anharmonic oscillator, we analogously choose the Hilbert space $L^2(\mathbb{R}, \mathrm{d}q)$. The quantum operators of the canonical variables q and P will be indicated by hats and shall act in the known way, similarly to the light oscillator. In order to make SAPT work at the technical level, we introduce the rescaled momentum operator $\hat{p} := \varepsilon \hat{P}$. Hence, the standard commutation relation of position and momentum operator becomes

$$[\hat{q}, \hat{p}]_\mathrm{s} = i\, \varepsilon\, \hat{\mathrm{I}}_\mathrm{s}, \tag{6.170}$$

and we choose the Weyl ordering prescription. The total Hilbert space is the topological tensor product

$$\mathcal{H} = L^2(\mathbb{R}, \mathrm{d}q) \otimes L^2(\mathbb{R}, \mathrm{d}x) \cong L^2(\mathbb{R}^2, \mathrm{d}q\, \mathrm{d}x). \tag{6.171}$$

Quantum operators on $\mathcal{H}$ have the form $\hat{A} \otimes \boldsymbol{B} \in \mathcal{B}(L^2_{\mathrm{s}}(\mathbb{R})) \otimes \mathcal{B}(L^2_{\mathrm{f}}(\mathbb{R}))$ for $\hat{A} \in \mathcal{B}(L^2_{\mathrm{s}}(\mathbb{R}))$ and $\boldsymbol{B} \in \mathcal{B}(L^2_{\mathrm{f}}(\mathbb{R}))$. The Hamilton operator $\hat{\boldsymbol{H}}$ associated with the classical Hamilton function H consequently has the form

$$\hat{\boldsymbol{H}} = \frac{\hat{p}^2}{2m} \otimes \mathbf{1}_{\mathrm{f}} + \hat{1}_{\mathrm{s}} \otimes \frac{\boldsymbol{y}^2}{2m} + \frac{1}{2}\, m\, \omega(\hat{q})^2 \otimes \boldsymbol{x}^2 \tag{6.172}$$

where we directly employed the rescaled momentum operator $\hat{p}$. Note that $\hat{\boldsymbol{H}}$ is *not* a bounded operator on the state space $\mathcal{H}$, but it is a well–defined bounded operator on $C^\infty_0(\mathbb{R}) \otimes C^\infty_0(\mathbb{R})$, i.e., on the topological tensor product of the spaces of smooth functions with compact support on $\mathbb{R}$.

Our first duty is then to check whether $\hat{\boldsymbol{H}}$ is essentially self–adjoint on a subspace of $\mathcal{H}$ in order to establish a well–defined quantum theory with a spectral calculus. For this purpose, a theorem which goes back to Kato (1972) is helpful. It states that if the potential energy contribution $V(q, x)$ in $H(q, P, x, y)$ is a measurable locally bounded function $V(q, x) \in L^\infty_{\mathrm{loc}}(\mathbb{R}^2)$, and if it is positive $V \geq 0$, then $\hat{\boldsymbol{H}}$ defined as an operator on $C^\infty_0(\mathbb{R}^2) \cong C^\infty_0(\mathbb{R}) \otimes C^\infty_0(\mathbb{R})$ is essentially self–adjoint. For our model, the potential energy function V is given by

$$V(q, x) = \frac{1}{2} m\, \omega_0^2 \left(1 + \frac{q^2}{L^2}\right)^2 \cdot x^2, \tag{6.173}$$

cf., equation (6.167). V is measurable, locally bounded, and positive. Consequently, $\hat{\boldsymbol{H}}$ is essentially self–adjoint on $C^\infty_0(\mathbb{R}^2)$ and hence, generates the time evolution of the quantum states in $\mathcal{H}$. To apply SAPT, we will now alter the representation of the heavy anharmonic quantum theory. We check the conditions that have to be met for SAPT and adapt the representation accordingly.

6.8.1. Checking of the Conditions and Preparations

We start by checking conditions (C1) to (C4) of SAPT referring to section 6.4.1. Regarding condition (C1), we note that the tensor product Hilbert space $\mathcal{H} = L^2(\mathbb{R}, \mathrm{d}q) \otimes L^2(\mathbb{R}, \mathrm{d}x)$ trivially satisfies (C1) because $L^2(\mathbb{R}, \mathrm{d}x)$ is a separable Hilbert space, and hence $\mathcal{H}$ has the required form of a tensor product. Recall that as $\mathcal{H}_{\mathrm{f}}$ is separable, it is possible to construct a unique isomorphism between the spaces $L^2(\mathbb{R}) \otimes \mathcal{H}_{\mathrm{f}}$ and $L^2(\mathbb{R}, \mathcal{H}_{\mathrm{f}})$ (Reed and Simon 1975a, Theorem II.10 on p.52). As remarked before, the $L^2(\mathbb{R}, \mathcal{H}_{\mathrm{f}})$ – representation of some state $\Psi \in \mathcal{H}$ gives rise to a Hilbert bundle picture: Therefore, consider $\mathcal{M} = \mathbb{R}$ as the base manifold of the Hilbert bundle $H \to \mathcal{M}$ for which every fibre is a Hilbert space $\mathcal{H}_{\mathrm{f}}$. A state $\Psi \in L^2(\mathbb{R}, \mathcal{H}_{\mathrm{f}})$ has the form of a section $\Psi : q \mapsto (q, \Psi(q)) \in H$ with $\Psi(q) \in \mathcal{H}_{\mathrm{f}}$. Regarding requirement (C2) which imposes conditions on the Hamilton operator, we start by representing the Hamilton operator as a symbol function, $\boldsymbol{H}(q, p)$, i.e.,

$$\boldsymbol{H}(q, p) = \frac{p^2}{2m} \mathbf{1}_{\mathrm{f}} + \frac{\boldsymbol{y}^2}{2m} + \frac{1}{2} m\, \omega(q)^2 \boldsymbol{x}^2 \tag{6.174}$$

which yields an unbounded operator on $L^2(\mathbb{R}, \mathrm{d}x)$ for every $(q, p) \in \mathbb{R}^2$. Following the space adiabatic perturbation scheme by Panati, Spohn, and Teufel (2003), $\boldsymbol{H}(q, p)$ must belong to one of the symbol classes $S^m_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. Consequently, it should have values in the space of *bounded* operators $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$, be a bounded function with respect to the slow configuration variable q, and be maximally polynomial with respect to the slow momentum p. It is clear that $\boldsymbol{H}$ cannot satisfy the

first of these conditions as the energy spectrum of the harmonic quantum oscillator is undoubtedly bounded from below but certainly not from above, hence it is not a bounded operator on $\mathcal{H}_\mathrm{f}$. The simplest solution would be to introduce a restricted domain $\mathcal{D}_{\boldsymbol{H}} \subset \mathcal{H}_\mathrm{f}$ on which $\boldsymbol{H}(q,p)$ is bounded.

We take a different path, however, because we want to closely follow Panati, Spohn, and Teufel (2003), for which we need symbols with values in the bounded operators on $\mathcal{H}_\mathrm{f}$. Our solution for this problem comes with an answer for the issue that the symbol function $\boldsymbol{H}(q,p)$ grows quadratically with respect to q while the symbol classes S^m_ρ require it to be bounded with respect to q. As it turns out, the fact that $\boldsymbol{H}(q,p)$ grows as well quadratically with respect to p will be problematic when considering condition (C4). Namely, the gap of our system is a constant gap such that the parameter γ of condition (C3) is zero. (C4) requires that in this case, the Hamilton symbol must be in S^0_ρ, i.e., a constant function with respect to p. Otherwise the adiabatic decoupling would not be uniform (Panati, Spohn, and Teufel 2003, p. 175).

Our strategy is the following: We define an auxiliary Hamilton symbol $\boldsymbol{H}_\mathrm{aux}(q,p)$ which is not only a bounded operator on $\mathcal{H}_\mathrm{f}$ but also a bounded function with respect to the slow phase space variables q and p. In order to define such an auxiliary Hamiltonian, it is helpful to rewrite the Hamilton symbol $\boldsymbol{H}(q,p)$ in its spectral form. Therefore, recall that it has the form of a harmonic oscillator Hamiltonian with a q–dependent frequency $\omega(q)$, mass m and an energy off–set $E_\mathrm{off}(p) := \frac{p^2}{2m}$. For any $(q,p) \in \mathbb{R}^2$, one can simply use the well–known solutions of the quantum harmonic oscillator which we denote by $\xi_n \in \mathcal{H}_\mathrm{f}$, $n \in \mathbb{N}$. Here, they depend on q and with their associated energy functions $E_n(q,p)$, the eigenvalue problem can be written in the form

$$\boldsymbol{H}(q,p)\,\xi_n(q) = E_n(q,p)\,\xi_n(q), \qquad E_n(q,p) := E_\mathrm{off}(p) + \omega(q)\left(n+\frac{1}{2}\right). \tag{6.175}$$

We emphasize that the eigenstates $\xi_n(q)$ are elements in $\mathcal{H}_\mathrm{f}$ and that the q–dependence is purely parametric. For a position representation on $\mathcal{H}_\mathrm{f} = L^2(\mathbb{R}, \mathrm{d}x)$, the $\xi_n(q)$ read

$$\xi_n(q,x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\,\omega(q)}{\pi}\right)^{1/4} e^{-\frac{m\omega(q)x^2}{2}}\, H_n\left(\sqrt{m\,\omega(q)}\,x\right) \tag{6.176}$$

where the H_n are the standard physicist's Hermite polynomials. Every eigenstate $\xi_n(q)$ gives rise to a q–dependent projection operator on $\mathcal{H}_\mathrm{f}$, namely

$$\boldsymbol{\pi}_n(q) := \xi_n(q)\,\langle \xi_n(q), \cdot\,\rangle_{\mathcal{H}_\mathrm{f}}. \tag{6.177}$$

As a consequence, the Hamiltonian symbol in its spectral form is given by

$$\boldsymbol{H}(q,p) = \sum_{n\geq 0} E_n(q,p)\,\boldsymbol{\pi}_n(q). \tag{6.178}$$

In a first step, let us define a cut–off Hamiltonian symbol $\boldsymbol{H}_N(q,p)$ which truncates the sum in (6.178) after some finite number $N \in \mathbb{N}$, i.e.,

$$\boldsymbol{H}_N(q,p) := \sum_{n=0}^{N} E_n(q,p)\,\boldsymbol{\pi}_n(q). \tag{6.179}$$

Obviously, $\boldsymbol{H}_N(q,p)$ has values in the bounded operators on $\mathcal{H}_\mathrm{f}$ due to the cut–off. Its norm is simply $E_N(q,p)$ which underlines that it still depends polynomially on q and p. Because the scheme requires a bounded Hamiltonian symbol in case of a constant gap to satisfy condition (C4), it is necessary to define the auxiliary Hamiltonian $\boldsymbol{H}_\mathrm{aux}(q,p)$ which satisfies all the requirements for SAPT. The idea is to replace the function $\boldsymbol{H}_N(q,p)$ by some appropriately bounded function outside a certain, compact region on the slow phase space. Therefore, let us define the interval $\Lambda := \{(q,p) : \|\boldsymbol{H}_N(q,p)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} < E_\mathrm{c}\}$ or more presicely all points $(q,p) \in \mathbb{R}^2$ for which it holds true that $E_N(q,p) < E_\mathrm{c}$. Therefore, we definitely need to choose $E_\mathrm{c} > \omega_0(N+1/2)$. Then, let us assume that it is possible to define the following auxiliary Hamiltonian symbol (Panati, Spohn, and Teufel 2003, p. 176)

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

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

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

In the given case, it is easy to construct such an auxiliary Hamiltonian. One simply extends the energy bands $E_n(q,p)$ outside the region $\Lambda + \epsilon$ smoothly by a set of bounded, smooth functions with appropriate transition conditions. For example, we can assume the representation of $\boldsymbol{H}_\mathrm{aux}(q,p)$ to be given by

$$\boldsymbol{H}_\mathrm{aux}(q,p) = \sum_{n=0}^{N} \tilde{E}_n(q,p)\,\boldsymbol{\pi}_n(q) \;\text{ with }\; \tilde{E}_n(q) = \begin{cases} E_n(q,p) & \text{if } (q,p) \in \Lambda + \epsilon, \\ b_n(q,p) & \text{if } (q,p) \notin \Lambda + \epsilon \end{cases} \tag{6.180}$$

where $b_n(q,p) \in C^\infty_\mathrm{b}(\mathbb{R}^2, \mathbb{R})$ is an appropriately bounded function for every $0 \leq n \leq N$. Besides, they must be pointwise distinct, i.e., they are not allowed to merge into or to cross with one another. This is important for the gap condition (C3). In fact, with these requirements $\boldsymbol{H}_\mathrm{aux}(q,p)$ satisfies (as we will show more explicitely in the sequel) all conditions for SAPT. It remains to show that the dynamics of $\hat{\boldsymbol{H}}_\mathrm{aux}$ and the original Hamiltonian agree on a set of relevant quantum states. Therefore, we first show that the dynamics of $\hat{\boldsymbol{H}}_N$ and $\hat{\boldsymbol{H}}_\mathrm{aux}$ coincide for states up to the cut–off energy E_c. To technically realize the proof, it is useful to resort to a new symbol class which falls under the generic definition 6.3 of symbol functions. The corresponding order function that we define is

$$\vartheta : \mathbb{R}^2 \to [0,\infty) : (q,p) \mapsto \alpha\,(1 + \beta\,q^2 + \delta\,p^2) \tag{6.181}$$

with $\alpha := \omega_0(N+1/2)$, $\beta := L^{-1}$ and $\delta := (2m\omega_0(N+1/2))^{-1}$ all bigger than zero. ϑ is constructed just to provide the symbol class $S(\vartheta, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ for the Hamiltonian $\boldsymbol{H}_N(q,p)$ as one can easily read off from definition 6.3. Next, we show that $\hat{\boldsymbol{H}}_N$ is essentially self–adjoint on the Schwartz space $\mathcal{S}(\mathbb{R}, \mathcal{H}_\mathrm{f})$ using a proposition by Dimassi and Sjöstrand (1999, p. 101) (see also in Teufel 2003, p. 208). To use the proposition, we need to demonstrate that the symbol function $(\boldsymbol{H}_N + i\mathbf{1}_\mathrm{f})$ is elliptic in the sense that $\|\boldsymbol{H}_N(q,p) + i\mathbf{1}_\mathrm{f}\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} \geq C\,\vartheta(q,p)$. Indeed, the spectral representation of $\boldsymbol{H}_N(q,p)$ makes it easy to deduce that

$$\|\boldsymbol{H}_N(q,p) + i\mathbf{1}_\mathrm{f}\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} = \sqrt{E_N(q,p)^2 + 1} > E_N(q,p) = \vartheta(q,p). \tag{6.182}$$

According to Dimassi and Sjöstrand (1999, Prop. 8.5), $\hat{\boldsymbol{H}}_N$ is then essentially self–adjoint on $\mathcal{S}(\mathbb{R}, \mathcal{H}_\mathrm{f})$.

This allows us in a second step to define a cut–off operator $\chi_{\mathrm{c}}(\hat{\boldsymbol{H}}_N)$ which projects on energies smaller than E_{c}. Therefore, consider the characteristic function $\chi_{\mathrm{c}} \in C_0^\infty(\mathbb{R})$ such that $\chi_{\mathrm{c}}|_{[0,E_{\mathrm{c}}]} = 1$ and $\chi_{\mathrm{c}}|_{[E_{\mathrm{c}}+\epsilon,\infty)} = 0$ for some small $\epsilon > 0$ (cf. Panati, Spohn, and Teufel 2003, p. 176). Then, according to Dimassi and Sjöstrand (1999) the operator–valued function $\chi_{\mathrm{c}}(\hat{\boldsymbol{H}}_N) \in \mathrm{OPS}^{-\infty}(\vartheta)$ obtained by the spectral calculus of self–adjoint operators is a smoothing operator. The associated symbol function $\boldsymbol{\chi}_{\mathrm{c}}(q,p) := \mathrm{Symb}(\chi_{\mathrm{c}}(\hat{\boldsymbol{H}}_N))$ has an asymptotic expansion which is $\mathbf{1}_{\mathrm{f}}$ on the interval Λ and equal to zero on the phase space region $\Lambda + \epsilon$. With the spectral projection operator $\hat{\mathbf{1}}_{(-\infty,E_{\mathrm{c}}]}$ on energies below E_{c}, it then follows that

$$(\hat{\boldsymbol{H}}_N - \hat{\boldsymbol{H}}_{\mathrm{aux}})\chi_{\mathrm{c}}(\hat{\boldsymbol{H}}_N) = \mathcal{O}_{-\infty}(\varepsilon^\infty), \quad (\hat{\boldsymbol{H}}_N - \hat{\boldsymbol{H}}_{\mathrm{aux}})\hat{\mathbf{1}}_{(-\infty,E_{\mathrm{c}}]}(\hat{\boldsymbol{H}}_N) = \mathcal{O}_0(\varepsilon^\infty) \tag{6.183}$$

where the second identity follows from the first one by using that $\chi_{\mathrm{c}}(\hat{\boldsymbol{H}}_N)\hat{\mathbf{1}}_{(-\infty,E_{\mathrm{c}}]}(\hat{\boldsymbol{H}}_N) = \hat{\mathbf{1}}_{(-\infty,E_{\mathrm{c}}]}(\hat{\boldsymbol{H}}_N)$. This suffices to show the equivalence of the dynamics generated by $\hat{\boldsymbol{H}}_N$ and $\hat{\boldsymbol{H}}_{\mathrm{aux}}$ up to infinitely small errors. In particular, it holds true that

$$\begin{aligned} &\left(e^{-i\hat{\boldsymbol{H}}_{\mathrm{aux}}t} - e^{-i\hat{\boldsymbol{H}}_N t}\right)\hat{\mathbf{1}}_{(-\infty,E_{\mathrm{c}}]}(\hat{\boldsymbol{H}}_N) \\ &\quad = -i\, e^{-i\hat{\boldsymbol{H}}_{\mathrm{aux}}t}\int_0^t \mathrm{d}s\, e^{i\hat{\boldsymbol{H}}_{\mathrm{aux}}s}(\hat{\boldsymbol{H}}_{\mathrm{aux}} - \hat{\boldsymbol{H}}_N)e^{-i\hat{\boldsymbol{H}}_N s}\,\hat{\mathbf{1}}_{(-\infty,E_{\mathrm{c}}]} \;=\; \mathcal{O}_0(\varepsilon^\infty|t|). \end{aligned} \tag{6.184}$$

Hence, we are able to construct an auxiliary Hamiltonian symbol $\boldsymbol{H}_{\mathrm{aux}}$ that satisfies all conditions (C1) to (C4) and which belongs to the symbol class $S_0^0(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. The dynamics generated by the Weyl quantization of this symbol approximates the dynamics of the cut–off Hamiltonian $\boldsymbol{H}_N$ according to the estimate in equation (6.184).

We stress however, that it is not possible to compare the dynamics of the auxiliary Hamiltonian to the dynamics generated by the original Hamiltonian, and which is due to the fact that the latter is an *unbounded* operator while the former is *bounded*. Consequently, one can pursue two different strategies now: Either, one uses the auxiliary Hamilton symbol for the application of SAPT in the following, and consequently obtains adiabatic perturbation series that are convergent. This is however at the price that the auxiliary Hamiltonian has different physical properties than the original Hamiltonian. *Or* one remains with the original Hamiltonian at the cost of possibly non–convergent perturbation series. In this thesis, we follow the latter approach. In other words, we use the rigorous mathematical framework that applies to the auxiliary system to *motivate* the adiabatic formulas for the actual unbounded system. The convergence of the resulting adiabatic series (say in the sense of matrix elements, i.e., the weak operator topology) then, however, has to be investigated by independent means in a case by case fashion, and might be rather difficult.

Now, before moving on to the actual application of the scheme we make a short comment regarding the physical interpretation of the scheme. The identification of a slow and a fast adiabatic subsystem typically becomes manifest by means of the adiabatic perturbation parameter $\varepsilon^2 := \frac{m}{M} \ll 1$. With the equipartition theorem and assuming that the system is ergodic, it follows that in thermal equilibrium the kinetic energy contributions of the light and the heavy oscillator must have the same phase space average and also the same time average, i.e.,

$$m\langle P^2\rangle \approx M\langle y^2\rangle, \text{ and consequently } \langle \dot{q}^2\rangle \approx \varepsilon^2\langle \dot{x}^2\rangle \tag{6.185}$$

where the angular brackets denote a phase space or a time average. Evidently, the heavy oscillator moves much slower in average than the light oscillator. Besides, we see that the momentum of the heavy oscillator is much larger than the momentum of the light oscillator, i.e., $\varepsilon^2\langle P^2\rangle \approx \langle y^2\rangle$. This motivates the above definition of the rescaled momentum $p := \varepsilon P$ such that $\langle p^2\rangle \approx \langle y^2\rangle$, and which gives rise to the perturbative treatment of the theory. The theory then requires that the Hamiltonian with the rescaled momenta p does *not* carry any inverse powers of ε which is indeed the case. We note that the fact that the average velocity of the heavy oscillator is much smaller than the average velocity of the light oscillator is independent of the frequencies of the two oscillators. Even if the frequency Ω_q of the heavy anharmonic oscillator was much larger than the frequency Ω_x of the light oscillator, it still holds true that the velocity of the heavy subsystem is much *smaller* than the velocity of the light oscillator (at least their time averages). This is possible because the amplitude A_x of the light oscillator can be much larger than the amplitude A_q of the heavy subsystem. Therefore, consider the relation between velocity and frequency of the two subsystems, namely $\dot{q} = A_q\,\Omega_q$, and $\dot{x} = A_x\,\Omega_x$. Then, with $\dot{q} \approx \varepsilon\dot{x}$ in time average coming from the equipartion theorem, it can still hold true that for example $\Omega_x = \varepsilon\Omega_q$ (i.e., the heavy oscillator frequency is much larger than the one of the light subsystem) by claiming that $A_q \approx \varepsilon^2 A_x$.

6.8.2. Space Adiabatic Construction Scheme

We are now ready to compute the second order effective Hamilton symbol $\boldsymbol{h}_{\mathrm{eff},(2),\mathrm{R}}$ for the oscillator toy model. We choose the quantum number $\nu \in \mathbb{N}$ associated with the fast harmonic oscillator. It suffices to compute the Moyal projector and the Moyal unitary up to *first* order in the perturbative construction scheme. We recall the form of the star product up to first order in ε for two smooth symbol functions $\boldsymbol{f}(q,p)$ and $\boldsymbol{g}(q,p)$ given by

$$(\boldsymbol{f} \star_\varepsilon \boldsymbol{g})(q,p) = (\boldsymbol{f}\cdot\boldsymbol{g})(q,p) + \frac{i\varepsilon}{2}\{\boldsymbol{f},\boldsymbol{g}\}_{\mathrm{s}}(q,p) + \mathcal{O}_0(\varepsilon^2). \tag{6.186}$$

Following the manual at the beginning of this section 6.5, we start with the construction of the Moyal projector.

(S1): Construction of the Projector Symbol $\boldsymbol{\pi}_{(1)}$

We expand the first order Moyal projector according to $\boldsymbol{\pi}_{(1)} = \boldsymbol{\pi}_0 + \varepsilon\,\boldsymbol{\pi}_1$. The zeroth order symbol arises naturally using the smooth eigenstate $\xi_\nu(q) \in \mathcal{H}_{\mathrm{f}}$ of the fast quantum oscillator, i.e., we choose

$$\boldsymbol{\pi}_0 := \boldsymbol{\pi}_\nu(q) = \xi_\nu(q)\,\langle \xi_\nu(q), \cdot\,\rangle_{\mathrm{f}}. \tag{6.187}$$

Note that the fast eigenstates, and hence the symbol $\boldsymbol{\pi}_0(q)$ depend solely on the fast configuration variable which will lead to significant simplifications for the space adiabatic construction scheme. To construct $\boldsymbol{\pi}_1(q,p)$, we first consider condition (S1–1) which determines the diagonal part of it.

Condition (S1–1): $\boldsymbol{\pi} \star_\varepsilon \boldsymbol{\pi} = \boldsymbol{\pi}$

By means of the series expansion of $\boldsymbol{\pi}_{(1)}$ and the star product in equation (6.186), we recall that (S1–1) yields up to first order

$$\boldsymbol{\pi}_0 \cdot \boldsymbol{\pi}_0 + \varepsilon \left(\frac{i}{2} \{\boldsymbol{\pi}_0, \boldsymbol{\pi}_0\}_{\mathrm{s}} + \boldsymbol{\pi}_0 \cdot \boldsymbol{\pi}_1 + \boldsymbol{\pi}_1 \cdot \boldsymbol{\pi}_0 \right) = \boldsymbol{\pi}_0 + \varepsilon \boldsymbol{\pi}_1 + \mathcal{O}_0(\varepsilon^2). \tag{6.188}$$

The zeroth order contributions yield the base requirement $\boldsymbol{\pi}_0 \cdot \boldsymbol{\pi}_0 = \boldsymbol{\pi}_0$ which holds true as a simple algebraic operator equation on $\mathcal{H}_{\mathrm{f}}$. The iterative construction scheme in section 6.7, and obviously equation (6.188) determine the diagonal contribution to $\boldsymbol{\pi}_1$ by requiring that

$$0 \stackrel{!}{=} \boldsymbol{a}_0 + \boldsymbol{\pi}_1 \cdot \boldsymbol{\pi}_0 + \boldsymbol{\pi}_0 \cdot \boldsymbol{\pi}_1 - \boldsymbol{\pi}_1 \quad \text{with} \quad \boldsymbol{a}_0 := \frac{i}{2} \{\boldsymbol{\pi}_0, \boldsymbol{\pi}_0\}_{\mathrm{s}}. \tag{6.189}$$

Since $\boldsymbol{\pi}_0(q)$ does not depend on p, the derivatives $\partial_p \boldsymbol{\pi}_0$ and hence the Poisson brackets for $\boldsymbol{a}_0$ vanish. Consequently, $\boldsymbol{a}_0$ vanishes and so does the diagonal part of $\boldsymbol{\pi}_1$, namely

$$\boldsymbol{\pi}_1^{\mathrm{D}} = -\boldsymbol{\pi}_0 \cdot \boldsymbol{a}_0 \cdot \boldsymbol{\pi}_0 + \boldsymbol{\pi}_0^{\perp} \cdot \boldsymbol{a}_0 \cdot \boldsymbol{\pi}_0^{\perp} = 0. \tag{6.190}$$

For determining the remaining off–diagonal part $\boldsymbol{\pi}_1^{\mathrm{OD}} := \boldsymbol{\pi}_1 - \boldsymbol{\pi}_1^{\mathrm{D}}$, we consider condition (S1–3).

Condition (S1–3): $\boldsymbol{H} \star_\varepsilon \boldsymbol{\pi} - \boldsymbol{\pi} \star_\varepsilon \boldsymbol{H} = 0$

We recall that the expansion of condition (S1–3) up to first order in ε yields

$$[\boldsymbol{H}_0, \boldsymbol{\pi}_0]_{\mathrm{f}} + \varepsilon \left(\frac{i}{2} \{\boldsymbol{H}_0, \boldsymbol{\pi}_0\}_{\mathrm{s}} - \frac{i}{2} \{\boldsymbol{\pi}_0, \boldsymbol{H}_0\}_{\mathrm{s}} + \boldsymbol{H}_0 \cdot \boldsymbol{\pi}_1 - \boldsymbol{\pi}_1 \cdot \boldsymbol{H}_0 \right) = \mathcal{O}_0(\varepsilon^2). \tag{6.191}$$

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

$$0 \stackrel{!}{=} -\boldsymbol{b}_0 + [\boldsymbol{H}_0, \boldsymbol{\pi}_1]_{\mathrm{f}} \quad \text{with} \quad \boldsymbol{b}_0 := \frac{i}{2} \left(\{\boldsymbol{H}_0, \boldsymbol{\pi}_0\}_{\mathrm{s}} - \{\boldsymbol{\pi}_0, \boldsymbol{H}_0\}_{\mathrm{s}} \right). \tag{6.192}$$

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

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

The concrete evaluation of the Poisson bracket in this equation necessitates the derivatives of $\boldsymbol{\pi}_0(q)$, and hence of the fast quantum states $\xi_n(q)$ with respect to q. We recall that the states $\xi_n(q)$ can be seen as smooth sections of a trivial Hilbert bundle $H = \Gamma_{\mathrm{s}} \times \mathcal{H}_{\mathrm{f}}$ where the slow phase space Γ_{s} identifies with the base manifold and $\mathcal{H}_{\mathrm{f}}$ is the fibre. The gauge potential $\boldsymbol{\mathcal{A}} \in C^\infty(\Lambda(\Gamma_{\mathrm{s}}) \otimes \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ is a one–form on Γ_{s} with values in the linear operators on $\mathcal{H}_{\mathrm{f}}$ and tells us how

the basis states $\xi_n(q)$ naturally change when moving on Γ_s. We want to identify its coefficients $\mathcal{A}_{qn}^{\ m}(q) \in C^\infty(\Gamma_s, \mathbb{R})$ for every n and $m \in \mathbb{N}$ with the partial derivatives of the states $\xi_n(q)$ with respect to q, in particular

$$(\boldsymbol{\mathcal{A}}\,\xi)_n(q) = \mathcal{A}_{qn}^{\ m}(q)\,\xi_m(q) \otimes \mathrm{d}q := \frac{\partial \xi_n(q)}{\partial q} \otimes \mathrm{d}q. \tag{6.193}$$

Therefore, recall that the states are harmonic quantum oscillator eigenstates with a q–dependent frequency $\omega(q)$, and a constant mass m, i.e., in Schrödinger representation, they have the form

$$\xi_n(q,x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\,\omega(q)}{\pi}\right)^{1/4} e^{-\frac{m\,\omega(q)\,x^2}{2}} H_n\left(\sqrt{m\,\omega(q)}\,x\right). \tag{6.194}$$

To continue, it is appropriate to use a representation in terms of the standard annihilation and creation operators which satisfy the commutation relation $[\,\boldsymbol{a}(q), \boldsymbol{a}^*(q)]_f = \mathbf{1}_f$ for every $q \in \mathbb{R}$, and which are given in terms of the fast canonical quantum operators $\boldsymbol{x}$ and $\boldsymbol{y}$ by

$$\boldsymbol{a}^*(q) = \sqrt{\frac{m\,\omega(q)}{2}} \left(\boldsymbol{x} - \frac{i}{m\,\omega(q)}\,\boldsymbol{y}\right). \tag{6.195}$$

The derivatives of $\xi_0(q)$ and $\boldsymbol{a}^*(q)$ with respect to q thus evaluate to

$$\frac{\partial \xi_0(q)}{\partial q} := \sqrt{2} f(q)\,\xi_2(q), \quad \frac{\partial \boldsymbol{a}^*(q)}{\partial q} := -2 f(q)\,\boldsymbol{a}(q), \tag{6.196}$$

where we defined the function $f(q) := -(\partial_q \omega)/(4\omega)$. Since the application of the creation operators $\boldsymbol{a}^*$ give rise to the excited state ξ_n by means of the relation $\xi_n = (\boldsymbol{a}^*)^n \xi_0/\sqrt{n!}$, it is easy to deduce the partial derivative of any state $\xi_n(q)$, and to read off the coefficients of the connection

$$\begin{aligned} \frac{\partial \xi_n(q)}{\partial q} &= -\sqrt{n(n-1)}\,f(q)\,\xi_{n-2}(q) + \sqrt{(n+1)(n+2)}\,f(q)\,\xi_{n+2}(q) \\ &=: \mathcal{A}_{qn}^{\ n-2}(q)\,\xi_{n-2}(q) + \mathcal{A}_{qn}^{\ n+2}(q)\,\xi_{n+2}(q), \end{aligned} \tag{6.197}$$

$$\text{i.e., } \mathcal{A}_{qn}^{\ n-2}(q) = -\sqrt{n(n-1)}\,f(q), \;\; \mathcal{A}_{qn}^{\ n+2}(q) = \sqrt{(n+1)(n+1)}\,f(q).$$

The only non–vanishing contributions $\mathcal{A}_{qn}^{\ n\pm2}$ of the connection relate states which mutually differ by two excitations. We recall that the derivative of the orthonormality relation $\langle \xi_n, \xi_m \rangle_f = \delta_{nm}$ with respect to q yields that

$$\mathcal{A}_{qn}^{\ n\pm2} = -\mathcal{A}_{q(n\pm2)}^{\ \ n}. \tag{6.198}$$

Moreover, we emphasize that the connection components in the direction of p vanish all identically because $\xi_n(q)$ does not depend on p for any $n \in \mathbb{N}$. With that we come back to the evaluation of $\boldsymbol{\pi}_1^{\mathrm{OD}}$ for which we need the symbol function $\partial_q \boldsymbol{\pi}_0$. In connection representation, it reads

$$\frac{\partial \boldsymbol{\pi}_0}{\partial q} = \mathcal{A}_{q\nu}^{\ \ m} \left(\xi_\nu \langle \xi_m, \cdot \rangle_f + \xi_m \langle \xi_\nu, \cdot \rangle_f\right). \tag{6.199}$$

The computation of $\boldsymbol{\pi}_1^{\mathrm{OD}}$ includes the term $\boldsymbol{\pi}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{H}_0 + E_\nu\,\mathbf{1}_f\}_s$ which we evaluate for illustrative purposes. First, we notice that we have only one non–vanishing contribution for the Poisson

bracket because $\partial_p \boldsymbol{\pi}_0$ is zero. What we get is

$$\begin{aligned}\boldsymbol{\pi}_0 \cdot \frac{\partial \boldsymbol{\pi}_0}{\partial q} \frac{\partial (\boldsymbol{H}_0 + E_\nu)}{\partial p} &= \xi_\nu \langle \xi_\nu, \cdot \rangle_{\mathrm{f}} \mathcal{A}_{q\nu}^{\ m} \left(\xi_\nu \langle \xi_m, \cdot \rangle_{\mathrm{f}} + \xi_m \langle \xi_\nu, \cdot \rangle_{\mathrm{f}} \right) \sum_n \frac{\partial (E_n + E_\nu)}{\partial p} \xi_n \langle \xi_n, \cdot \rangle_{\mathrm{f}} \\ &= \sum_{n \neq \nu} \mathcal{A}_{q\nu}^{\ n} \frac{\partial (E_n + E_\nu)}{\partial p} \xi_\nu \langle \xi_n, \cdot \rangle_{\mathrm{f}}. \end{aligned} \tag{6.200}$$

Note that the p–derivative of $\boldsymbol{H}_0 + E_\nu \mathbf{1}_0$ only applies to the energy functions $E_n + E_\nu$ because the states do not depend on p. Besides, we used that $\mathcal{A}$ does not have any diagonal contributions, i.e., $\mathcal{A}_{q\nu}^{\ \nu} = 0$. The evaluation of $\{\boldsymbol{H}_0 + E_\nu \mathbf{1}_{\mathrm{f}}, \boldsymbol{\pi}_0\}_{\mathrm{f}} \cdot \boldsymbol{\pi}_0$ works completely analogous. Finally, to obtain $\boldsymbol{\pi}_1^{\mathrm{OD}}$ we multiply by a factor $(\boldsymbol{H}_0^{\perp} - E_\nu \mathbf{1}_{\mathrm{f}})^{-1}$ from the left and the right respectively. For the first contribution, this yields

$$\boldsymbol{\pi}_0 \cdot \frac{\partial \boldsymbol{\pi}_0}{\partial q} \frac{\partial (\boldsymbol{H}_0 + E_\nu)}{\partial p} \cdot (\boldsymbol{H}_0^{\perp} - E_\nu \mathbf{1}_{\mathrm{f}})^{-1} = \sum_{n \neq \nu} \frac{\mathcal{A}_{q\nu}^{\ n}}{E_n - E_\nu} \frac{\partial (E_n + E_\nu)}{\partial p} \xi_\nu \langle \xi_n, \cdot \rangle_{\mathrm{f}}. \tag{6.201}$$

Recalling that the energy band functions are given for this model by $E_n(q,p) = \frac{p^2}{2m} + \omega(q)\left(n + \frac{1}{2}\right)$, the total expression for $\boldsymbol{\pi}_1^{\mathrm{OD}} = \boldsymbol{\pi}_1$ yields

$$\boldsymbol{\pi}_1 = \frac{ip}{2m\omega} \left(\mathcal{A}_{q\nu}^{\ \nu-2} \left(\xi_\nu \langle \xi_{\nu-2}, \cdot \rangle_{\mathrm{f}} - \xi_{\nu-2} \langle \xi_\nu, \cdot \rangle_{\mathrm{f}} \right) + \mathcal{A}_{q\nu}^{\ \nu+2} \left(\xi_{\nu+2} \langle \xi_\nu, \cdot \rangle_{\mathrm{f}} - \xi_\nu \langle \xi_{\nu+2}, \cdot \rangle_{\mathrm{f}} \right) \right). \tag{6.202}$$

In particular, we used that the operator $\partial_p(\boldsymbol{H}_0 + E_\nu \mathbf{1}_{\mathrm{f}})$ is simply $(2p/m) \cdot \mathbf{1}_{\mathrm{f}}$ and that the inverse of $(\boldsymbol{H}_0^{\perp} - E_\nu \mathbf{1}_{\mathrm{f}})$ reduces to a factor, $(E_{\nu\pm2} - E_\nu)^{-1} = \pm(2\omega)^{-1}$ when projected on $\xi_{\nu\pm2}$. These are in fact the only contributions because the only non–vanishing connection coefficients are

$$\mathcal{A}_{q\nu}^{\ \nu-2}(q) = -f(q)\sqrt{\nu(\nu-1)}, \quad \mathcal{A}_{q\nu}^{\ \nu+2}(q) = f(q)\sqrt{(\nu+1)(\nu+2)}, \tag{6.203}$$

$$f(q) = -\frac{1}{4\omega(q)} \frac{\partial \omega(q)}{\partial q} = -\frac{q}{2(L^2 + q^2)}. \tag{6.204}$$

Condition (S1–2): $\boldsymbol{\pi}^* = \boldsymbol{\pi}$

It is easy to check that $\boldsymbol{\pi}_{(1)}$ satisfies condition (S1–2) up to first order in the perturbative scheme by transposing and complex conjugating $\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}_1$. We see that this improved projection symbol maps from and to further fast energy states, not only from and to ξ_ν, which shows that the totally invariant projector $\boldsymbol{\pi}$ will probably involve an infinite number of fast energy states. A mapping to a simpler reference space appears thus to be very helpful.

(S2): Construction of the Unitary Symbol $\boldsymbol{u}_{(1)}$

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

$$\boldsymbol{\pi}_{\mathrm{R}} := \xi_\nu(q_0) \left\langle \xi_\nu(q_0), \cdot \right\rangle_{\mathrm{f}} =: \zeta_\nu \langle \zeta_\nu, \cdot \rangle_{\mathrm{f}}. \tag{6.205}$$

In order to mediate between $\mathcal{K}_\mathrm{f}$ and the subspace associated with $\boldsymbol{\pi}$, we introduce the Moyal unitary up to first order $\boldsymbol{u}_{(1)} = \boldsymbol{u}_0 + \varepsilon \boldsymbol{u}_1$. It makes sense to choose

$$\boldsymbol{u}_0(q) := \sum_n \zeta_n \left\langle \xi_n(q), \cdot \right\rangle_\mathrm{f} \tag{6.206}$$

as initial data of the iteration. We split $\boldsymbol{u}_1$ into a hermitian and an antihermitian part $\boldsymbol{h}_1 = \boldsymbol{h}_1^*$ and $\boldsymbol{k}_1 = -\boldsymbol{k}_1^*$ such that $\boldsymbol{u}_{(1)} := \boldsymbol{u}_0 + \varepsilon(\boldsymbol{h}_1 + \boldsymbol{k}_1) \cdot \boldsymbol{u}_0$.

Conditions (S2–1) and (S2–2): $\boldsymbol{u} \star_\varepsilon \boldsymbol{u}^* = \mathbf{1}_f = \boldsymbol{u}^* \star_\varepsilon \boldsymbol{u}$

The unitarity condition (S2–1) becomes up to first order in terms of the symbol $\boldsymbol{h}_1$

$$\boldsymbol{u}_0 \cdot \boldsymbol{u}_0^* - \mathbf{1}_\mathrm{f} + \varepsilon \left(\frac{i}{2} \{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_\mathrm{s} + 2\boldsymbol{h}_1 \right) = \mathcal{O}_0(\varepsilon^2), \tag{6.207}$$

and likewise for the second condition (S2–2). At zeroth order, the resulting conditions $\boldsymbol{u}_0 \cdot \boldsymbol{u}_0^* - \mathbf{1}_\mathrm{f} = 0$, and $\boldsymbol{u}_0^* \cdot \boldsymbol{u}_0 - \mathbf{1}_\mathrm{f} = 0$ are trivially satisfied for the choice of $\boldsymbol{u}_0$ in (6.206). Regarding the condition at first order in ε that arises from (6.207), it is clear that the Poisson bracket $\{\boldsymbol{u}_0, \boldsymbol{u}_0^*\}_\mathrm{s}$ vanishes since $\boldsymbol{u}_0$ does not depend on p. It therefore follows directly that $\boldsymbol{h}_1 = 0$. The antihermitian part $\boldsymbol{k}_1$ is determined by condition (S2–3).

Condition (S2–3): $\boldsymbol{u} \star_\varepsilon \boldsymbol{\pi} \star_\varepsilon \boldsymbol{u}^* = \boldsymbol{\pi}_R$

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

$$\boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}_0^* - \boldsymbol{\pi}_\mathrm{R} + \varepsilon \left([\boldsymbol{k}_1, \boldsymbol{\pi}_\mathrm{R}]_\mathrm{f} + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1 \cdot \boldsymbol{u}_0^* \right) = \mathcal{O}_0(\varepsilon^2). \tag{6.208}$$

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

$$\boldsymbol{u}_1 = \left[\boldsymbol{\pi}_\mathrm{R}, \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1^\mathrm{OD} \cdot \boldsymbol{u}_0^*\right]_\mathrm{f} \cdot \boldsymbol{u}_0. \tag{6.209}$$

Using the already known solution for $\boldsymbol{\pi}_1^\mathrm{OD}$, this gives in terms of the connection coefficients and the eigenstates

$$\boldsymbol{u}_1 = \frac{ip}{2m\omega} \left(\mathcal{A}_{q\nu}^{\nu-2} \left(\zeta_\nu \langle \xi_{\nu-2}, \cdot \rangle_\mathrm{f} + \zeta_{\nu-2} \langle \xi_\nu, \cdot \rangle_\mathrm{f} \right) - \mathcal{A}_{q\nu}^{\nu+2} \left(\zeta_{\nu+2} \langle \xi_\nu, \cdot \rangle_\mathrm{f} + \zeta_\nu \langle \xi_{\nu+2}, \cdot \rangle_\mathrm{f} \right) \right). \tag{6.210}$$

(S3): Construction of the Effective Hamilton Symbol $\boldsymbol{h}_{\mathit{eff},(2),R}$

The last step of the perturbation scheme consists in pulling the dynamics of the chosen subspace associated with $\boldsymbol{\pi}$ to the ε–independent subspace $\hat{\boldsymbol{\pi}}_\mathrm{R}\mathcal{H}$. This essentially means that by applying the unitary operator $\hat{\boldsymbol{U}} = \hat{\boldsymbol{u}} + \mathcal{O}_0(\varepsilon^\infty)$ to the Hamiltonian $\hat{\boldsymbol{H}}_0$, the action of the latter on elements in $\hat{\boldsymbol{\Pi}}\mathcal{H}$ is rotated to $\hat{\boldsymbol{\pi}}_\mathrm{R}\mathcal{H}$. The effective Hamiltonian $\hat{\boldsymbol{h}}_\mathrm{eff}$ which acts on this subspace is the Weyl

quantization of the symbol $\boldsymbol{h}_{\text{eff}}$ which is determined by condition (S3), namely by $\boldsymbol{h}_{\text{eff}} = \boldsymbol{u} \star_\varepsilon \boldsymbol{H}_0 \star_\varepsilon \boldsymbol{u}^*$. Again, we assume an ansatz of a formal power series $\boldsymbol{h}_{\text{eff},(2)} = \boldsymbol{h}_{\text{eff},0} + \varepsilon\, \boldsymbol{h}_{\text{eff},1} + \varepsilon^2\, \boldsymbol{h}_{\text{eff},2}$. In the following, we restrict our attention directly to the subspace associated with $\boldsymbol{\pi}_{\text{R}}$ and project on it. At zeroth order, the condition (S3) gives

$$\boldsymbol{h}_{\text{eff},0,\text{R}} = \boldsymbol{\pi}_{\text{R}} \cdot \boldsymbol{u}_0 \cdot \boldsymbol{H}_0 \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\text{R}} = \left(\frac{p^2}{2m} + \omega(q) \left(\nu + \frac{1}{2} \right) \right) \boldsymbol{\pi}_{\text{R}} \tag{6.211}$$

which corresponds to a standard Born–Oppenheimer result: it includes the original kinetic energy contribution of the slow oscillator plus an effective potential energy due to its interaction with the fast oscillator. For the first and second order contributions in (S3), we recall that it is useful to star multiply the condition by $\boldsymbol{u}$ from the right to minimize the computational effort. This yields

$$\boldsymbol{u} \star_\varepsilon \boldsymbol{H}_0 - \boldsymbol{h}_{\text{eff},0} \star_\varepsilon \boldsymbol{u} = \varepsilon\, \boldsymbol{h}_{\text{eff},1} \star_\varepsilon \boldsymbol{u} + \mathcal{O}_0(\varepsilon^2) = \varepsilon\, \boldsymbol{h}_{\text{eff},1} \cdot \boldsymbol{u} + \mathcal{O}_0(\varepsilon^2) \tag{6.212}$$

for determining the first order contribution $\boldsymbol{h}_{\text{eff},1}$, and leads to

$$\boldsymbol{h}_{\text{eff},1} = \left(\boldsymbol{u}_1 \cdot \boldsymbol{H}_0 - \boldsymbol{h}_{\text{eff},0} \cdot \boldsymbol{u}_1 + \frac{i}{2} \{\boldsymbol{u}_0, \boldsymbol{H}_0\}_{\text{s}} - \frac{i}{2} \{\boldsymbol{h}_{\text{eff},0}, \boldsymbol{u}_0\}_{\text{s}} \right) \cdot \boldsymbol{u}_0^*. \tag{6.213}$$

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

$$\boldsymbol{h}_{\text{eff},1,\text{R}} = \frac{i}{2} \boldsymbol{\pi}_{\text{R}} \cdot \{\boldsymbol{u}_0, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\text{R}} = 0. \tag{6.214}$$

The same strategy applies for deriving $\boldsymbol{h}_{\text{eff},2,\text{R}}$ which is however non–vanishing. Its determining equation is given here by

$$\begin{aligned} \boldsymbol{h}_{\text{eff},2,\text{R}} &= \frac{i}{2} \boldsymbol{\pi}_{\text{R}} \cdot \left[\{\boldsymbol{u}_1, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} - \boldsymbol{h}_{\text{eff},1} \cdot \boldsymbol{u}_1 - \frac{i}{2} \{\boldsymbol{h}_{\text{eff},1}, \boldsymbol{u}_0\}_{\text{s}} \right] \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\text{R}} \\ &= \frac{i}{2} \{\boldsymbol{\pi}_{\text{R}} \cdot \boldsymbol{u}_1, \boldsymbol{H}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\text{R}} \end{aligned} \tag{6.215}$$

where the second line follows from observing that $\boldsymbol{\pi}_{\text{R}} \cdot \boldsymbol{h}_{\text{eff},1} = 0$. To evaluate the symbol in equation (6.215), we use the explicit representation of the symbol in terms of connections and eigenstates introduced in section 6.7, and then that any of the $\mathcal{A}_{pn}^{\ m}$ vanishes as well as that $(E_n - E_\nu)$ does not depend on p. This yields

$$\begin{aligned} \boldsymbol{h}_{\text{eff},2,\text{R}} &= \left[\frac{1}{2} \frac{\partial E_n}{\partial p} \frac{A_{\nu n} \mathcal{A}_{q\nu}^{\ n}}{E_\nu - E_n} + \frac{1}{4} \frac{\partial}{\partial p} \left[\frac{A_{\nu n}}{E_\nu - E_n} \right] (E_\nu - E_n) \mathcal{A}_{q\nu}^{\ n} \right] \boldsymbol{\pi}_{\text{R}} \\ &= \left[\frac{\partial E_n}{\partial p} \right]^2 \left[\frac{(\mathcal{A}_{q\nu}^{\ \nu-2})^2}{E_\nu - E_{\nu-2}} + \frac{(\mathcal{A}_{q\nu}^{\ \nu+2})^2}{E_\nu - E_{\nu+2}} \right] \boldsymbol{\pi}_{\text{R}} + \frac{1}{2} \frac{\partial^2 E_n}{\partial p^2} \left[(\mathcal{A}_{q\nu}^{\ \nu-2})^2 + (\mathcal{A}_{q\nu}^{\ \nu+2})^2 \right] \boldsymbol{\pi}_{\text{R}}. \end{aligned} \tag{6.216}$$

Then inserting the explicit expressions for the energies and the coefficients of the connections, we obtain

$$\boldsymbol{h}_{\text{eff},2,\text{R}} = \frac{L^2}{2m\,\omega_0} \left[-\frac{p^2 q^2}{m \left(L^2 + q^2 \right)^3} \left(\nu + \frac{1}{2} \right) + \frac{q^2}{\left(L^2 + q^2 \right)^2} \frac{\omega_0}{2L^2} \left(\nu^2 + \nu + 1 \right) \right] \boldsymbol{\pi}_{\text{R}}. \tag{6.217}$$

The second order contribution $\boldsymbol{h}_{\text{eff},2,\text{R}}$ displays the effects of non–adiabaticity. We see that this second order contribution does not only give an additional potential term which solely depends on q as a backreaction from the light harmonic oscillator onto the heavy oscillator. It also includes a kinetic term which depends on the momentum p. This last line will serve as the starting point for a further analysis of the solutions to this effective Hamilton operator.

6.8.3. Approximate Solutions to the Effective Hamiltonian

We start with the evaluation of the zeroth order symbol of equation (6.211). It is easy to evaluate the action of its quantization on some generic tensor product wave function in $\mathcal{H} = \mathcal{H}_\text{s} \otimes \mathcal{H}_\text{f}$: The operator associated with the fast subsystem $\boldsymbol{\pi}_\text{R}$ has the eigenfunction ζ_ν which is the same for every $(q,p) \in \Gamma_\text{s}$. Thus, one can simply examine the action of the (q,p)–dependent energy function on elements of $\mathcal{H}_\text{s}$. The Schrödinger equation for some generic wave function $\psi^0_\nu \in \mathcal{H}_\text{s}$, derived from the Hamilton symbol in equation (6.211), is given by

$$\left(-\frac{\partial_q^2}{2M} + \frac{1}{2}M\Omega_\nu^2 q^2\right)\psi^0_{d,\nu}(q) = \tilde{E}_{d,\nu}\psi^0_{d,\nu}(q) \tag{6.218}$$

where we defined

$$\Omega_\nu = \sqrt{\frac{2\omega_0}{ML^2}\left(\nu+\frac{1}{2}\right)}, \;\; \tilde{E}_{d,\nu} = E_{d,\nu} - \omega_0\left(\nu+\frac{1}{2}\right), \tag{6.219}$$

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

$$E_{d,\nu} = \omega_0\left(\nu+\frac{1}{2}\right) + \sqrt{\frac{2\omega_0}{ML^2}\left(\nu+\frac{1}{2}\right)}\cdot\left(d+\frac{1}{2}\right). \tag{6.220}$$

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

The contribution to the effective Hamilton operator of second order $\hat{\boldsymbol{h}}_{\text{eff},2,\text{R}}$ is the Weyl quantization of the symbol function in equation (6.216). As this operator represents a perturbation of the zeroth order Hamiltonian $\hat{\boldsymbol{h}}_{\text{eff},0,\text{R}}$, standard quantum mechanical perturbation theory applies and provides corrections to the spectrum $\{E_{d,\nu}\}_{d\in\mathbb{N}}$. Namely, the shift of the energy due to $\hat{\boldsymbol{h}}_{\text{eff},2,\text{R}}$ is given as the expectation value in the zeroth order states, i.e., $\Delta E_{d,\nu} := \langle \psi^0_{d,\nu}, \hat{\boldsymbol{h}}_{\text{eff},2,\text{R}}\psi^0_{d,\nu}\rangle_\text{s}$. Knowing both ingredients, the zeroth order states and the form of the perturbation effective Hamiltonian, it is straightforward to compute $\Delta E_{d,\nu}$ for any d and ν in $\mathbb{N}$. We present the derivations and the explicit formulae in Appendix B and content ourselves with providing the expression for $\Delta E_{0,\nu}$ for

illustration here. Therefore, we define a dimensionless parameter $\ell_\nu := \sqrt{M\Omega_\nu}\, L$ and we obtain

$$\Delta E_{0,\nu} = -\frac{\Omega_\nu}{4}(\nu^2+\nu+1) + \frac{\Omega_\nu^2}{16\omega_0}\left(\nu+\frac{1}{2}\right)(2+7\ell_\nu^2+2\ell_\nu^4) \tag{6.221}$$
$$+ \mathrm{Erf}(\ell_\nu)\frac{\sqrt{\pi}e^{\ell_\nu^2}}{8\ell_\nu}\left(\frac{\Omega_\nu^2(\nu+\frac{1}{2})}{4\,\omega_0}(11\ell_\nu^2-2+20\ell_\nu^4+4\ell_\nu^6) - \Omega_\nu(\nu^2+\nu+1)(1+2\ell_\nu^2)\right)$$

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

As a final remark, we note that the second order effective Hamilton operator in (6.216) contains inverse powers of q. Since the model here allows for the use of standard quantum mechanical perturbation theory, it is possible to extract relevant information of the quantum problem using perturbation theory. This is a very specific case and is due to the fact that the zeroth order solutions of the effective Hamiltonian admit a discrete spectrum. As we will see below, the cosmological models yield effective Hamilton constraints at zeroth order with *continuous* spectrum such that the standard perturbative methods are no longer available. It is however possible to define a dense and invariant domain on which these operators are well–defined.

Part III.

Quantum Cosmology with Backreaction

7. Homogeneous and Isotropic Cosmology

In this chapter, we apply SAPT to a simple cosmological model. Its main purpose is to illustrate the formalism for a constrained gravitational system which allows for a discussion of some challenges that we will encounter in the inhomogeneous models hereafter. After introducing the system, we apply SAPT to this system in section 7.1. In section 7.2, we explain the challenges occuring in SAPT for quantum cosmology. This chapter relies to a large extent on (Neuser, Schander, and Thiemann 2019) and (Schander and Thiemann 2019a).

7.1. Presentation of the System and Preparations

We consider Einstein general relativity reduced to spatial homogeneity and isotropy at the classical level, including a cosmological constant $\Lambda \in \mathbb{R}^+$ and coupled to a spatially homogeneous, isotropic and real Klein–Gordon field ϕ with mass $m \in \mathbb{R}^+$. The model rests on a four–dimensional space time manifold $\mathcal{M}$ which we assume to be globally hyperbolic. The gravitational field g has Lorentzian signature $(-,+,+,+)$ and space time $(\mathcal{M}, g)$ is a pseudo–Riemannian manifold. According to a theorem by Geroch (1970), a globally hyperbolic manifold necessarily has the topology $\mathcal{M} \cong \mathbb{R} \times \sigma$ where σ is a fixed three–dimensional manifold of arbitrary topology. In the following, we choose σ to be the compact, flat three–torus $\mathbb{T}^3$ with side lengths l in all directions. We emphasize that the torus actually comprises *any* compact and flat manifold since they are all finitely covered by tori according to a theorem by Bieberbach (Bieberbach 1911, 1912). Accordingly, we set the cosmological curvature parameter to $k = 0$. We choose coordinates such that the time parameter t labels the homogeneous and isotropic spatial slices. The metric tensor g of general relativity has the time–dependent scale factor a as its only remaining dynamical degree of freedom. The scalar field reduces to a homogeneous and isotropic time–dependent field $\phi : \mathbb{R} \to \mathbb{R}$. The Einstein–Hilbert and the matter field cosmological action are given by

$$S[a,\phi] = \int_{\mathbb{R}} \mathrm{d}t \left(-\frac{1}{2\kappa} \left(6\,\dot{a}^2 a + 2\,\Lambda\, a^3 \right) + \frac{1}{2\lambda} a^3 \left(\dot{\phi}^2 - m^2 \phi^2 \right) \right) \tag{7.1}$$

where a dot denotes a derivative with respect to cosmic time t, and the integration over the torus volume produces a factor $l^3 \equiv 1$. Here, κ and λ are the coupling constants of general relativity and the Klein–Gordon system respectively where $\kappa = 8\pi G$ and G is Newton's constant, and we set $\hbar \equiv 1 \equiv c$ throughout this chapter. If both a and ϕ are dimensionless, as we assume, then both coupling constants have the same dimension. Thus, it is reasonable to define the adiabatic perturbation parameter as the dimensionless ratio

$$\varepsilon^2 := \frac{\kappa}{\lambda}. \tag{7.2}$$

Note that we can associate mass parameters to the coupling constants, namely $m_\lambda^2 := \lambda^{-1}$ and $M_{\mathrm{Pl}}^2 := \kappa^{-1}$ where M_{Pl} is the Planck mass. We assume that $m_\lambda \ll M_{\mathrm{Pl}}$ and thus $\varepsilon \ll 1$ which is certainly the case if m_λ is in the mass range of a typical standard model particle. It transpires that in the adiabatic language, gravity is the "slow" sector and the Klein–Gordon particle the "fast" one. This may seem counterintuitive when one interprets the Klein–Gordon field as an inflaton candidate and the inflationary phase when ϕ practically freezes (for small m) while a expands exponentially. However, note that the distinction of slow and fast degrees of freedom uses intrinsically a statistical average over phase space. For instance, when the system under consideration has a true Hamiltonian bounded from below, one uses the equipartition theorem. In our case we do not have a true Hamiltonian but rather a Hamilton constraint such that the equipartition theorem does not apply. Section 7.2.1 explains that the Hamilton constraint itself gives rise to conditions under which the scheme satisfies the standard physical intuition of slow and fast sectors.

The space adiabatic scheme requires a Hamiltonian formulation of the problem. We define the conjugate momenta of a and ϕ as $p_a := \varepsilon \frac{\partial L}{\partial \dot{a}}$ and $\mu := \frac{\partial L}{\partial \dot{\phi}}$ where L is the Lagrange function associated with the action $S = \int \mathrm{d}t\, L$. The Poisson brackets of the canonical variables evaluate to $\{a, p_a\} = \varepsilon$ and $\{\phi, \mu\} = 1$. The Legendre transformation generates the Hamilton constraint

$$C(a, p_a, \phi, \mu) := -\frac{1}{12}\frac{p_a^2}{a} + \frac{\Lambda}{\lambda\kappa}a^3 + \frac{\mu^2}{2a^3} + \frac{1}{2\lambda^2}m^2 a^3 \phi^2 \tag{7.3}$$

where for notational reasons, we divided the whole constraint by a constant factor λ. For simplifying the analysis by means of SAPT, we switch to triad–like canonical variables

$$b := \pm\sqrt{a^3}, \quad \rho := \frac{2}{3}\frac{p_a}{\sqrt{a}} \tag{7.4}$$

which is a double cover of the original phase space. Note that the range of b consists of two branches, a positive and a negative one. We do not restrict to any of these. Hence, the slow phase space associated with the geometry is $\Gamma_{\mathrm{s}} = \mathbb{R}^2$ and the fast phase space is $\Gamma_{\mathrm{f}} = \mathbb{R}^2$. In order to keep the notation as simple as possible, we introduce the following parameters and functions

$$m_{\mathrm{G}} := \frac{8}{3}, \quad \omega_{\mathrm{G}}^2 := \frac{3\Lambda}{4\lambda\kappa}, \quad \tilde{m} := b^2, \quad \omega_{\mathrm{KG}}^2 := \frac{m^2}{\lambda^2}. \tag{7.5}$$

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

$$C(b, \rho, \phi, \mu) = -\frac{\rho^2}{2\,m_{\mathrm{G}}} + \frac{1}{2}m_{\mathrm{G}}\omega_{\mathrm{G}}^2 b^2 + \frac{\mu^2}{2\tilde{m}(b)} + \frac{1}{2}\tilde{m}(b)\omega_{\mathrm{KG}}^2\phi^2. \tag{7.6}$$

We quantize the system and start by considering the scalar field subsystem. We choose a standard L^2–Hilbert space, and denote it by $\mathcal{H}_{\mathrm{f}} = L^2(\mathbb{R}, \mathrm{d}\phi)$. The quantum operators are indicated as bold letters, and the scalar field operator and its conjugate momentum satisfy the canonical commutation relation $[\boldsymbol{\phi}, \boldsymbol{\mu}]_{\mathrm{f}} = i\,\mathbf{1}_{\mathrm{f}}$. Similarly, the state space of the geometrical subsystem will be denoted by $\mathcal{H}_{\mathrm{s}} = L^2(\mathbb{R}, \mathrm{d}b)$. The quantum operators wear hats and the canonical commutation relation for the geometrical variable and its conjugate momentum are $[\hat{b}, \hat{\rho}]_{\mathrm{s}} = i\,\varepsilon\,\hat{1}_{\mathrm{s}}$. The quantum theory of the coupled system has the tensor product Hilbert space $\mathcal{H}_{\mathrm{s}} \otimes \mathcal{H}_{\mathrm{f}}$. Another possible choice of rep-

resentation is for example used in LQC (Ashtekar, Bojowald, and Lewandowski 2003b; Ashtekar, Pawlowski, and P. Singh 2006b; Bojowald 2008) for which one motivation is that inverse powers of a or b can be made well–defined following the technique introduced for LQG (Thiemann 1996, 1998). That technique does not work in the presently chosen Schrödinger representation, and we will come back to the problem of choosing a suitable domain on which the resulting Hamiltonian is well–defined. Formally, the constraint operator on the tensor product Hilbert space is given by

$$\hat{\boldsymbol{C}} = \left(-\frac{\hat{\rho}^2}{2m_{\mathrm{G}}} + \frac{1}{2}m_{\mathrm{G}}\,\omega_{\mathrm{G}}^2\,\hat{b}^2\right) \otimes \mathbf{1}_{\mathrm{f}} + \frac{1}{2\,\tilde{m}(\hat{b})} \otimes \boldsymbol{\mu}^2 + \frac{1}{2}\tilde{m}(\hat{b})\,\omega_{\mathrm{KG}}^2 \otimes \boldsymbol{\phi}^2. \tag{7.7}$$

This operator is neither a bounded operator on $\mathcal{H}_{\mathrm{f}}$ nor on $\mathcal{H}_{\mathrm{s}}$, even worse, it is not bounded from below due to the constraint character of general relativity. If one were to solve the associated quantum mechanical problem, the goal would be to find quantum states within $\mathcal{H}$ that are annihilated by the constraint operator $\hat{\boldsymbol{C}}$. As far as we know, there are no solutions known to this problem. In what follows, we perform a systematic step by step SAPT treatment that will allow us to derive a much simpler quantum mechanical problem which approximates the above problem up to a desired error estimate.

7.1.1. Checking of the Conditions and Preparations

We check the conditions (C1) – (C4) from section 6.4.1 for the cosmological model. Condition (C1) holds without further ado since the cosmological Hilbert space $\mathcal{H}_{\mathrm{s}} \otimes \mathcal{H}_{\mathrm{f}}$ has the required tensor product form. In addition, $\mathcal{H}_{\mathrm{s}}$ is an L^2–space and $\mathcal{H}_{\mathrm{f}}$ is a separable Hilbert space. Following condition (C2), we represent the quantum constraint (7.7) as a symbol function $\boldsymbol{C}(b,\rho)$ with values in the linear operators on the Klein–Gordon Hilbert space $\mathcal{H}_{\mathrm{f}}$. Formally, we simply quantize the Klein–Gordon subsystem by means of a standard Weyl quantization procedure and obtain

$$\boldsymbol{C}(b,\rho) = \left(-\frac{\rho^2}{2m_{\mathrm{G}}} + \frac{1}{2}m_{\mathrm{G}}\omega_{\mathrm{G}}^2 b^2\right)\mathbf{1}_{\mathrm{f}} + \frac{\boldsymbol{\phi}^2}{2\,\tilde{m}(b)} + \frac{1}{2}\tilde{m}(b)\omega_{\mathrm{KG}}^2\,\boldsymbol{\mu}^2. \tag{7.8}$$

This symbol function is an unbounded linear operator on $\mathcal{H}_{\mathrm{f}}$ for every $(b,\rho) \in \mathbb{R}^2$. In particular, the operator corresponds to the Hamiltonian of a quantum harmonic oscillator with constant frequency ω_{KG}, b–dependent mass $\tilde{m}(b)$, and an off–set energy. As such, the symbol has for fixed, finite (b,ρ) an energy spectrum which is bounded from below but not from above. Besides, $\boldsymbol{C}(q,p)$ is an unbounded function with respect to both b and ρ. According to SAPT, the constraint symbol must however belong to one of the symbol classes $S_\rho^m(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ in order to give a uniformly convergent error estimate (m should not be confused here with the mass parameter). More precisely, the symbol should have values in the space of *bounded* operators on $\mathcal{H}_{\mathrm{f}}$, be a bounded function with respect to b and maximally grow polynomially in ρ.

By means of the standard quantum oscillator eigensolutions $\xi_n \in \mathcal{H}_{\mathrm{f}}$, $n \in \mathbb{N}$, for the described oscillator with b–dependent mass, the corresponding eigenvalue equation has the form

$$\boldsymbol{C}(b,\rho)\,\xi_n(b) = E_n(b,\rho)\,\xi_n(b), \quad E_n(b,\rho) = -\frac{\rho^2}{2m_{\mathrm{G}}} + \frac{1}{2}m_{\mathrm{G}}\omega_{\mathrm{G}}^2 b^2 + \omega_{\mathrm{KG}}\left(n+\frac{1}{2}\right). \tag{7.9}$$

We emphasize that the b–dependence of the states is purely parametric. As in the oscillator ex-

ample, it is evident to define a b–dependent projection operator on $\mathcal{H}_{\mathrm{f}}$

$$\boldsymbol{\pi}_n(b) := \xi_n(b)\,\langle \xi_n(b), \cdot\,\rangle_{\mathcal{H}_{\mathrm{f}}} \tag{7.10}$$

by means of which the Hamilton symbol constraint has the spectral representation

$$\boldsymbol{C}(b,\rho) = \sum_{n\geq 0} E_n(b,\rho)\,\boldsymbol{\pi}_n(b). \tag{7.11}$$

In order to respect the conditions for the application of SAPT, it is possible to define an auxiliary Hamilton symbol $\boldsymbol{H}_{\mathrm{aux}}(b,\rho)$ in close analogy to the oscillator example. In a first step, one defines the symbol $\boldsymbol{C}_N(b,\rho)$ by cutting the sum in equation (7.11) after the $N+1$'st contribution. $\boldsymbol{C}_N$ lies in the symbol class with order function $\vartheta : \mathbb{R}^2 \to \mathbb{R} : (b,\rho) \mapsto C\cdot(1+\alpha\, b^2+\beta\,\rho^2)$ where C, α, $\beta \in \mathbb{R}^+$ are appropriate positive constants. $\boldsymbol{C}_N(b,\rho)$ lies consequently in $S(\vartheta, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. Besides it has values in the self–adjoint operators and is elliptic, the proofs for this being analogous to the ones for the oscillator model. Then, by restricting the norm of $\boldsymbol{C}_N(b,\rho)$ to a certain cut–off value C_{c} and defining an associated domain Λ in the slow phase space, it is possible to define the cut–off operator $\chi_{\mathrm{c}}(\hat{\boldsymbol{C}}_N) \in \mathcal{B}(\mathcal{H})$. The domain Λ also suggests to define the auxiliary Hamilton symbol $\boldsymbol{C}_{\mathrm{aux}}$, which agrees with $\boldsymbol{C}_N$ on Λ and smoothly transforms into a bounded function outside this domain, cf. (Panati, Spohn, and Teufel 2003, p. 176). The construction yields that

$$\big(\hat{\boldsymbol{C}}_{\mathrm{aux}} - \hat{\boldsymbol{C}}_N\big)\,\hat{\mathbf{1}}_{(-\infty,C_{\mathrm{c}}]} = \mathcal{O}_0(\varepsilon^\infty), \tag{7.12}$$

and we refer to the previous chapter for more details. Since we are solely interested in the solutions to the constraint (i.e., there is no absolute time propagation), this statement suffices for our purposes. The theory hence allows us to perform the space adiabatic scheme with $\boldsymbol{C}_{\mathrm{aux}}$ whose solutions are very close to solutions of the cut–off constraint $\boldsymbol{C}_N$. We stress however that this does not guarantee that these solutions are close to the solutions of the original Hamilton constraint $\hat{\boldsymbol{C}}$. A statement similar to equation (7.12) with $\hat{\boldsymbol{C}}_N$ replaced by the original constraint $\hat{\boldsymbol{C}}$ does not hold since $\hat{\boldsymbol{C}}$ is an unbounded operator. As for the oscillator model, one can now either proceed by applying SAPT to the auxiliary constraint which guarantees a convergent adiabatic perturbation theory but which is physically different from the original problem. The convergence (e.g., with respect to the weak operator topology) must then be investigated by independent means, and which might be a non–trivial enterprise. On the other hand, one may continue with the original constraint, leading to a possibly non–convergent perturbation series. Here, we follow the second strategy.

7.1.2. Space Adiabatic Construction Scheme

Again, we proceed in three steps to compute an effective Hamilton constraint $\boldsymbol{C}_{\mathrm{eff},(2),\mathrm{R}}$.

(S1): Construction of the Projector Symbol $\boldsymbol{\pi}_{(1)}$

With the power series ansatz $\boldsymbol{\pi}_{(1)} = \boldsymbol{\pi}_0 + \varepsilon\,\boldsymbol{\pi}_1$, and the natural choice for the base clause

$$\boldsymbol{\pi}_0 := \xi_\nu(b)\,\langle \xi_\nu(b), \cdot\,\rangle_{\mathcal{H}_\mathrm{f}} \tag{7.13}$$

for some fixed fast quantum number $\nu \in \mathbb{N}$, we construct the symbol function $\boldsymbol{\pi}_{(1)}(b,\rho)$ in close analogy to the considerations of the oscillator model. Similarly, the first condition (S1–1), $\boldsymbol{\pi} \star_\varepsilon \boldsymbol{\pi} = \boldsymbol{\pi}$, yields that the diagonal contribution to $\boldsymbol{\pi}_1$ vanishes because $\boldsymbol{\pi}_0(b)$ depends solely on b. Regarding the third condition (S1–3), $\boldsymbol{C}_0 \star_\varepsilon \boldsymbol{\pi} - \boldsymbol{\pi} \star_\varepsilon \boldsymbol{C}_0 = 0$, recall that it yields

$$\begin{aligned}\boldsymbol{\pi}_1 = &-\frac{i}{2}\,\boldsymbol{\pi}_0 \cdot \{\boldsymbol{\pi}_0, \boldsymbol{C}_0 + E_\nu\,\mathbf{1}_\mathrm{f}\}_\mathrm{s} \cdot (\boldsymbol{C}_0^\perp - E_\nu\,\mathbf{1}_\mathrm{f})^{-1} \cdot \boldsymbol{\pi}_0^\perp \\ &-\frac{i}{2}\,(\boldsymbol{C}_0^\perp - E_\nu\,\mathbf{1}_\mathrm{f})^{-1} \cdot \boldsymbol{\pi}_0^\perp \cdot \{\boldsymbol{C}_0 + E_\nu\,\mathbf{1}_\mathrm{f}, \boldsymbol{\pi}_0\}_\mathrm{s} \cdot \boldsymbol{\pi}_0\end{aligned} \tag{7.14}$$

as a determining equation for $\boldsymbol{\pi}_1$ where we defined $\boldsymbol{C}_0^\perp = \boldsymbol{C}_0 \cdot \boldsymbol{\pi}_0^\perp$. To evaluate the partial derivative $\partial_b \boldsymbol{\pi}_0$ in this equation, we need to evaluate the derivative of the states $\xi_n(b) \in \mathcal{H}_\mathrm{f}$ as well as the derivatives of the canonically defined creation and annihilation operators $\boldsymbol{a}^*(b) \in \mathcal{L}(\mathcal{H}_\mathrm{f})$ and $\boldsymbol{a}(b) \in \mathcal{L}(\mathcal{H}_\mathrm{f})$. Therefore, recall that the initial, fast eigenvalue problem with solutions $\xi_n(b)$ coincides with the quantum harmonic oscillator problem with a generalized b–dependent mass $\tilde{m}_\mathrm{KG}(b) = b^2$ and an (b,ρ)–dependent off–set energy. Accordingly, the creation operator $\boldsymbol{a}^*(b)$ can be written in terms of the canonical pair $(\boldsymbol{\phi}, \boldsymbol{\mu})$ as

$$\boldsymbol{a}(b)^* = \sqrt{\frac{\tilde{m}(b)\omega_\mathrm{KG}}{2}}\left(\boldsymbol{\phi} - \frac{i}{\tilde{m}(b)\omega_\mathrm{KG}}\boldsymbol{\mu}\right). \tag{7.15}$$

The derivatives of the vacuum state $\xi_0(b)$ and the creation operator are given by

$$\frac{\partial \xi_0}{\partial b} := \sqrt{2} f(b)\,\xi_2(b), \quad \frac{\partial \boldsymbol{a}(b)^*}{\partial b} = -2 f(b)\,\boldsymbol{a}(b) \tag{7.16}$$

where we introduced the function $f(b) := -(\partial_b \tilde{m})/(4\tilde{m}) = -1/(2b)$. We propose the definition of a covariant derivative or more precisely of a gauge potential $\boldsymbol{\mathcal{A}}$ associated with the b–derivative of the fast oscillator states. Using the natural basis choice from above, its coefficients with respect to the b–direction on Γ_s are given by

$$\frac{\partial \xi_n(b)}{\partial b} = \mathcal{A}_{bn}{}^{n-2}(b)\,\xi_{n-2}(b) + \mathcal{A}_{bn}{}^{n+2}(b)\,\xi_{n+2}(b) \tag{7.17}$$

with $\mathcal{A}_{bn}{}^{k}(b) = -\sqrt{n(n-1)}\,f(b)\,\delta_n^{k+2} + \sqrt{(n+1)(n+2)}\,f(b)\,\delta_n^{k-2}$. All coefficients $\mathcal{A}_{\rho n}{}^{m}$ in the ρ–direction vanish because the fast eigenstates do not depend on ρ. As for the oscillator model, only the coefficients of the gauge potential that connect states differing by two excitations are non–vanishing as can be read off from the above assignment. Since we have real–valued eigenstates, the connection coefficients are real–valued, too such that the orthonormality relation between the fast states yields that $\mathcal{A}_{bn}{}^{m} = -\mathcal{A}_{bm}{}^{n}$. The b–derivative of the projector symbol $\boldsymbol{\pi}_0$ follows from using Riesz' representation and we can simply write

$$\frac{\partial \boldsymbol{\pi}_0}{\partial b} = \mathcal{A}_{b\nu}{}^{m}\,(\xi_\nu \langle \xi_m, \cdot\,\rangle_\mathrm{f} + \xi_m \langle \xi_\nu, \cdot\,\rangle_\mathrm{f}) \tag{7.18}$$

where we emphasize that ν is a fixed quantum number while m (of course not to be confused with the mass of the Klein–Gordon field) runs over all natural numbers. To evaluate $\boldsymbol{\pi}_1$, we use that the partial derivative $\partial_\rho\,(\boldsymbol{C}_0 + E_\nu \cdot \mathbf{1}_\mathrm{f})$ is simply $(-2\rho/m_\mathrm{G}) \cdot \mathbf{1}_\mathrm{f}$ because only the spectral functions $E_n(b,\rho)$ depend on ρ while the states do not. The functional form of the energy functions also reduces $(\boldsymbol{C}_0^\perp - E_\nu)$ to a factor $\pm(2\omega_\mathrm{KG})^{-1}$. As a result, the projector symbol $\boldsymbol{\pi}_1$ has the form

$$\boldsymbol{\pi}_1 = -\frac{i\rho}{2m_\mathrm{G}\omega_\mathrm{KG}}\big(\mathcal{A}_{b\nu}^{\ \nu-2}\,(\xi_\nu\langle\xi_{\nu-2},\cdot\,\rangle_\mathrm{f} - \xi_{\nu-2}\langle\xi_\nu,\cdot\,\rangle_\mathrm{f}) + \mathcal{A}_{b\nu}^{\ \nu+2}\,(\xi_{\nu+2}\langle\xi_\nu,\cdot\,\rangle_\mathrm{f} - \xi_\nu\langle\xi_{\nu+2},\cdot\,\rangle_\mathrm{f})\big)\,. \tag{7.19}$$

With this, one can easily check that $\boldsymbol{\pi}_{(1)}$ satisfies all three conditions subsumed under (S1) up to first order in ε, i.e., that it is a projector and commutes with the full Hamiltonian up to errors of order ε^2.

(S2): Construction of the Unitary Symbol $\boldsymbol{u}_{(1)}$

Analogously to the proceeding in section 6.8.2, we construct a unitary symbol $\boldsymbol{u}_{(1)}$ which maps the dynamical subspace related to $\boldsymbol{\pi}_{(1)}$ to a suitable reference subspace $\mathcal{K}_\mathrm{f} \subset \mathcal{H}_\mathrm{f}$. We select one fixed $(b_0,\rho_0) \in \Gamma_\mathrm{s}$ and define the reference projection by

$$\boldsymbol{\pi}_\mathrm{R} := \xi_\nu(b_0)\,\big\langle\xi_\nu(b_0),\cdot\,\big\rangle_\mathrm{f} =: \zeta_\nu\langle\zeta_\nu,\cdot\,\rangle_\mathrm{f}. \tag{7.20}$$

A natural choice for the unitary operator in line with conditions (S2) at zeroth order is given by

$$\boldsymbol{u}_0(b) = \sum_{n\geq 0}\zeta_n\,\big\langle\xi_n(b),\cdot\,\big\rangle_\mathrm{f}. \tag{7.21}$$

The iterative construction gives in analogy to the results in section 6.8.2 for $\boldsymbol{u}_1$ that

$$\begin{aligned}\boldsymbol{u}_1 &= [\boldsymbol{\pi}_\mathrm{R}, \boldsymbol{u}_0\cdot\boldsymbol{\pi}_1^\mathrm{OD}\cdot\boldsymbol{u}_0^*]_\mathrm{f}\cdot\boldsymbol{u}_0 \\ &= \frac{i\rho}{2\,m_\mathrm{G}\,\omega_\mathrm{KG}}\big[\mathcal{A}_{b\nu}^{\ \nu-2}\,(\zeta_\nu\langle\xi_{\nu-2},\cdot\,\rangle_\mathrm{f} + \zeta_{\nu-2}\langle\xi_\nu,\cdot\,\rangle_\mathrm{f}) - \mathcal{A}_{b\nu}^{\ \nu+2}(\zeta_{\nu+2}\langle\xi_\nu,\cdot\,\rangle_\mathrm{f} + \zeta_\nu\langle\xi_{\nu+2},\cdot\,\rangle_\mathrm{f})\big],\end{aligned} \tag{7.22}$$

recalling that the hermitian part of the unitary symbol simply vanishes because, again, the states do not depend on ρ.

(S3): Construction of the Effective Constraint Symbol $\boldsymbol{C}_{\mathit{eff},(2),R}$

We restrict the computation of the effective Hamiltonian to the selected reference space, i.e., we compute $\boldsymbol{C}_{\mathrm{eff},(2),\mathrm{R}}(b,\rho) := \boldsymbol{\pi}_\mathrm{R}\cdot\boldsymbol{C}_{\mathrm{eff},(2)}(b,\rho)\cdot\boldsymbol{\pi}_\mathrm{R}$. The zeroth order contribution of this symbol is given according to condition (S3) by

$$\boldsymbol{C}_{\mathrm{eff},0,\mathrm{R}}(b,\rho) = \left(-\frac{\rho^2}{2m_\mathrm{G}} + \frac{1}{2}m_\mathrm{G}\omega_\mathrm{G}^2 b^2 + \omega_\mathrm{KG}\left(\nu+\frac{1}{2}\right)\right)\boldsymbol{\pi}_\mathrm{R}. \tag{7.23}$$

Thus, the effective constraint symbol for the gravitational degrees of freedom includes the bare gravitational constraint symbol plus an off–set energy which stems from the Klein–Gordon particle's chosen energy band. This result corresponds to the Born–Oppenheimer approximation. As

in the oscillator model, the first order contribution of the effective constraint symbol $\boldsymbol{C}_{\text{eff},1}(b,\rho)$ contains only off-diagonal terms such that $\boldsymbol{C}_{\text{eff},1,\text{R}}(b,\rho)$ vanishes identically, namely

$$\boldsymbol{C}_{\text{eff},1,\text{R}}(b,\rho) = \frac{i}{2}\{\boldsymbol{\pi}_{\text{R}}\cdot\boldsymbol{u}_0, \boldsymbol{C}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}}\cdot\boldsymbol{u}_0^*\cdot\boldsymbol{\pi}_{\text{R}} = 0. \tag{7.24}$$

The same reasoning applies to the computation of $\boldsymbol{C}_{\text{eff},2,\text{R}}(b,\rho)$ which is thus given by

$$\begin{aligned}\boldsymbol{C}_{\text{eff},2,\text{R}} &= \frac{i}{2}\{\boldsymbol{\pi}_{\text{R}}\cdot\boldsymbol{u}_1, \boldsymbol{C}_0 + E_\nu \mathbf{1}_{\text{f}}\}_{\text{s}}\cdot\boldsymbol{u}_0\cdot\boldsymbol{\pi}_{\text{R}} \\ &= \left[\frac{\partial E_n}{\partial\rho}\right]^2\left[\frac{(\mathcal{A}_{b\nu}{}^{\nu-2})^2}{E_\nu - E_{\nu-2}} + \frac{(\mathcal{A}_{b\nu}{}^{\nu+2})^2}{E_\nu - E_{\nu+2}}\right]\boldsymbol{\pi}_{\text{R}} + \frac{1}{2}\frac{\partial^2 E_n}{\partial\rho^2}\left[(\mathcal{A}_{b\nu}{}^{\nu-2})^2 + (\mathcal{A}_{b\nu}{}^{\nu+2})^2\right]\boldsymbol{\pi}_{\text{R}}.\end{aligned} \tag{7.25}$$

Finally, we insert the explicit results for the energy functions and the connection coefficients and obtain

$$\boldsymbol{C}_{\text{eff},2,\text{R}}(b,\rho) = -\frac{1}{2\,m_{\text{G}}}\left(\frac{\rho^2}{m_{\text{G}}\omega_{\text{KG}}b^2}\left(\nu+\frac{1}{2}\right) + \frac{1}{2b^2}\left(\nu^2+\nu+1\right)\right)\boldsymbol{\pi}_{\text{R}}. \tag{7.26}$$

This proves our statement that besides the trivial Born–Oppenheimer approximation further back-reaction effects arise for the gravitational subsystem. It is now easy to evaluate the action of this symbol on some generic tensor product wave function in $\mathcal{H} = \mathcal{H}_{\text{s}}\otimes\mathcal{H}_{\text{f}}$ since the Klein–Gordon tensor factor does not depend on the gravitational degrees of freedom anymore. The effective problem reduces to a quantum problem with respect to the slow geometric sector only.

One can start to analyze the quantum problem by considering only the zeroth order Hamilton constraint (7.23). It corresponds to the problem of an inverted harmonic oscillator with mass m_{G}, frequency ω_{G} and an off–set energy $E_{\text{off},\nu} := \omega_{\text{KG}}(\nu+1/2)$. Solutions to this problem are well–known and it turns out that the corresponding spectrum is of the continuous type (Finster and Isidro 2017). To see this, let us perform a canonical transformation by a simple rescaling in order to obtain the new variables

$$x := \sqrt{\omega_{\text{G}} m_{\text{G}}}\,b, \quad y := \frac{\rho}{\sqrt{\omega_{\text{G}} m_{\text{G}}}}. \tag{7.27}$$

Inserting these variables and multiplying the constraint $C_{\text{eff},0,\text{R}}(b,\rho)$ by $2/\omega_{\text{G}}$ gives the new constraint defined by

$$C_0(x,y) := -y^2 + x^2 + \tilde{E}_{\text{off},\nu} \tag{7.28}$$

where $\tilde{E}_{\text{off},\nu} := 2E_{\text{off},\nu}/\omega_{\text{G}}$. For the quantum theory of the inverted oscillator, we employ a standard Schrödinger representation and use $L^2(\mathbb{R},\mathrm{d}x)$ as a Hilbert space. One can show that the corresponding quantum operator

$$\hat{C}_0 = \frac{\partial^2}{\partial x^2} + x^2 + \tilde{E}_{\text{off},\nu} \tag{7.29}$$

has the domain of definition $C^\infty(\mathbb{R})\cap L^2(\mathbb{R})$, and is essentially self–adjoint on $C_0^\infty(\mathbb{R})\subset L^2(\mathbb{R})$ (Reed and Simon 1975b, Theorems X.36 and X.38). Its (generalized) spectral problem has hence the form

$$\left(\frac{\partial^2}{\partial x^2} + x^2 + \tilde{E}_{\text{off},\nu}\right)\psi_\lambda(x) = E_\lambda\psi_\lambda(x) \tag{7.30}$$

where $E_\lambda \in \mathbb{R}$ is real–valued and associated with a quantum number λ. As it turns out, the spectrum is continuous and so λ can also take continuous values. In fact, let $\lambda = -(1/2)(1 - iE_\lambda)$. Then, the two linearly independent generalized eigensolutions $\psi_\lambda(x)$ associated with the spectral value E_λ are given by (Finster and Isidro 2017)

$$\psi_\lambda(x) = \exp\left(\frac{i}{2}x^2\right) H_\lambda\left(e^{i\frac{3\pi}{4}}\right), \quad \psi_{-(\lambda+1)}(x) = \exp\left(-\frac{i}{2}x^2\right) H_{-(\lambda+1)}\left(e^{i\frac{5\pi}{4}}\right) \tag{7.31}$$

where for $\lambda \in \mathbb{C} \setminus \mathbb{N}$, the Hermite functions $H_\lambda(z)$ are given according to Lebedev (1972)

$$H_\lambda(z) = \frac{1}{2\Gamma(-\lambda)} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \Gamma\left(\frac{n-\lambda}{2}\right) (2z)^n. \tag{7.32}$$

These solutions are also known as parabolic cylinder functions. They are not normalizable as functions in $L^2(\mathbb{R}, \mathrm{d}x)$ (Finster and Isidro 2017), and therefore can only serve as a generalized eigenbasis. The spectrum is also continuous. However, since the operator $\hat{C}_0$ is essentially self–adjoint, the generalized eigenvectors of parabolic cylinder functions are complete (Gel'fand and N. Y. Vilenkin 1964, p. 126). Hence, one can construct any normalizable combination of parabolic cylinder functions which are however no eigensolutions to the problem. A thorough construction of wavepackets that are sharply peaked in energy, and coherent states that follow classical trajectors can be found in (Barton 1986).

In the next step, one would like to solve the perturbed problem including the corrections at second order SAPT. For this purpose, it would be desirable to take advantage of the known solutions to the zeroth order problem, and use a quantum mechanical perturbation theory, similar to the usual perturbation theory employed for the oscillator model in the previous chapter. Unfortunately, this method is applicable only when the zeroth order has a pure point spectrum, which is obviously not the case here (Neuser, Schander, and Thiemann 2019). As we explain in this paper, the perturbation theory for absolutely continuous operators is very unstable in the sense that a perturbation by an operator of arbitrarily small Hilbert–Schmidt norm exists such that their sum has pure point spectrum (Kato 1995). We are not aware of any rigorous work in that direction and it seems that the spectral problem of the Hamilton constraint operator including zeroth and second order contributions cannot use simple perturbative methods but must be addressed by independent methods.

7.2. Challenges for the Space Adiabatic Scheme

7.2.1. Identification of Slow and Fast Sectors

For the cosmological model, it would be helpful to have a physical intuition about the respective behavior of the slow and fast subsystems. In this section, we will provide such an intuition based on the considerations in (Schander and Thiemann 2019a).

In case of the oscillator toy model, and more generally for unconstrained dynamical systems, one resorts to the equipartition theorem in order to show that the heavy subsystem has a much smaller rate of change than the light subsystem (see for example equation (6.185)). However,

the equipartition theorem is not applicable in the case of unconstrained cosmological systems. Therefore, consider the statistical average of some phase space function $f \in C^\infty(\Gamma)$ on the full phase space $\Gamma = \Gamma_s \times \Gamma_f$, and let H be the Hamiltonian of the system. Let us denote the phase space variables in analogy to the previous section by (a, p_a, ϕ, μ). The phase space average of f is then defined by

$$\langle f \rangle := \frac{1}{Z} \int_\Gamma \mathrm{d}a\, \mathrm{d}p_a\, \mathrm{d}\phi\, \mathrm{d}\mu\, e^{-\beta H} f(a, p_a, \phi, \mu), \quad Z := \int_\Gamma \mathrm{d}a\, \mathrm{d}p_a\, \mathrm{d}\phi\, \mathrm{d}\mu\, e^{-\beta H}$$

where Z is the partition function and $\beta := (k_B T)^{-1}$ is the reciprocal of the thermodynamic temperature of the system. For $\langle f \rangle$ to make sense, we must assume that H is bounded from below such that the integrals converge. This also assures that in the integration by parts that one performs to show that $\langle p_a \frac{\partial H}{\partial p_a} \rangle = \beta^{-1}$ no boundary terms appear. Both conditions are violated for the cosmological model because the gravitational kinetic energy is negative. However, we have the constraint itself and two highly differing parameters, namely the gravitational coupling constant κ and the matter coupling constant λ of the scalar field, and which give rise to the perturbation parameter $\varepsilon^2 = \frac{\kappa}{\lambda}$. The existence of the perturbative parameter assures that we can safely apply the space adiabatic formalism but one might question the physical relevance of its use. In order to see under which conditions the theory leads to a physical distinction of slow and fast sectors, we take a closer look at the constraint. We use the Hamilton constraint from the previous section but stick to the more intuitive scale factor variable for the geometric subsystem. By multiplying with the global factor λ^{-1}, we obtain

$$\frac{1}{12} \frac{\varepsilon^2 P_a^2}{a} = \frac{\Lambda}{\lambda^2 \varepsilon^2} a^3 + \frac{\mu^2}{2a^3} + \frac{1}{2\lambda} m^2 a^3 \phi^2 \tag{7.33}$$

where we defined the canonical momentum of the geometric subsystem according to $P_a := \frac{\partial L}{\partial \dot{a}}$. The typical quantity to measure the velocity of the expansion of the Universe is the Hubble parameter $H := \frac{\dot{a}}{a}$ which we rather denote by v_H in order to avoid confusion with the Hamilton function. It is related to the variables (a, P_a) according to $v_H = -\varepsilon^2 \frac{\lambda}{6} \frac{P_a}{a^2}$. Likewise, the velocity of the scalar field is given by $v_\phi := \dot{\phi} = \lambda \frac{\mu}{a^3}$. Inserting this in the constraint (7.33) gives

$$v_H^2 = \frac{1}{6} \varepsilon^2 v_\phi^2 + \frac{1}{3} \Lambda + \frac{1}{6} \varepsilon^2 m^2 \phi^2. \tag{7.34}$$

A comparison of the respective terms allows for the conclusion that for small cosmological constant and small potentials of the scalar field, we have indeed that the geometric velocity is much smaller than the velocity of the scalar field, namely $v_H \sim \varepsilon v_\phi$, at least at a classical level. Accordingly, the homogeneous mode of the scalar field can be identified as the fast sector while the geometry appears as the slow subsystem owing to our assumption on κ and λ. Indeed, we have that $v_H \ll v_\phi$.

During a possible inflationary phase however, we know that the scalar field potential must be much larger than the kinetic term, i.e., $v_H^2 \approx \frac{1}{6} \varepsilon^2 m^2 \phi^2 \gg \frac{1}{6} \varepsilon^2 v_\phi^2$, assuming that the cosmological constant is negligibly small. One might introduce another perturbative parameter $\delta \ll 1$ that quantifies the ratio between v_H^2 and the kinetic contribution of the scalar field, for example, $\delta^2 v_H^2 \sim \varepsilon^2 v_\phi^2$, and hence $v_H \sim \frac{\varepsilon}{\delta} v_\phi$. In the case that $\varepsilon \ll \delta$, we can still establish that $v_H \ll v_\phi$, and hence

the physical intuition of the slow geometric system and the fast scalar field remains valid. There is however the possibility that $\varepsilon \geq \delta$, in which case we obtain that $v_H \geq v_\phi$. SAPT then still works at the technical level as long as $\varepsilon \ll 1$ but the classical picture that associates the geometry with the slow subsystem fails.

7.2.2. Non–Polynomial Operators

The Hamilton constraint $C(b, \rho, \phi, \mu)$ from equation (7.6) is non–polynomial in the scale factor related configuration variable b and contains inverse powers of it. The same is true for the geometric part of the effective Hamilton constraint $C_{\text{eff},(2),\text{R}}(b, \rho, \phi, \mu)$ that arises from the results in equations (7.23) and (7.26) by omitting the fast projector $\boldsymbol{\pi}_\text{R}$. Moreover, we must assume that in higher orders of the space adiabatic scheme even higher inverse contributions of the geometric phase space variables occur. This is because the connection coefficients are proportional to b^{-1}. As we will see in the following sections, for more involved models also the momenta ρ can enter with inverse orders in the effective Hamilton constraint. It hence transpires that it would be desirable to have a dense set of vectors which is invariant under *any* of the operators corresponding to b^i and ρ^j for $i, j \in \mathbb{Z}$. In LQC (as also discussed in (Schander and Thiemann 2019a)), one deals with negative powers of b by using a non–standard representation inspired by the representation used in the full LQG theory such that the spectrum of b is pure point rather than absolutely continuous. Hence, the commutator between fractional powers of b and Weyl elements of ρ is both densely defined and introduces the desired negative powers of b. This comes at the price that the operator corresponding to ρ does not exist and one consequently needs to approximate it by polynomials in Weyl elements. However, negative powers of ρ would then also need to be approximated by inverse polynomials of Weyl elememts and these are not in the domain of b 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 represenation. The advantage would be that the operators corresponding to b and ρ exist. Indeed, one can establish the following result as found and stated in (Schander and Thiemann 2019a):

Theorem 7.1. Domain for Non–Polynomial Operators
Consider the canonical pair of position and momentum operators $(\hat{q}, \hat{p})$ and use a Schrödinger representation on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}, \mathrm{d}x)$, i.e., $(\hat{q}\psi)(x) = x\psi(x)$, $(\hat{p}\,\psi)(x) = -i\,\mathrm{d}\psi(x)/\mathrm{d}x$ for $\psi \in \mathcal{H}$. Then, the following holds true:

1. There exists a dense and invariant domain $\mathcal{D} \subset \mathcal{H}$ for the operators $\hat{q}^{\,i}$ and $\hat{p}^{\,j}$ where $i \in \mathbb{Z}$ and $j \in \mathbb{N}_0$. This domain $\mathcal{D}$ consists of smooth functions of rapid decrease both at $x = 0$ and at $x = \pm\infty$.
2. The domain $\mathcal{D}$ is spanned by functions $\{\xi_n(x)\}$ with $n \in \mathbb{Z}$ whose inner products can be computed analytically in closed form. Correspondingly, an orthonormal basis can be constructed by means of the Gram–Schmidt procedure.
3. Let $f(x)$ be a function such that both, $f(x)$ and $f^{-1}(x)$ are polynomially bounded and smooth except possibly at $x = 0$ or $x \pm \infty$. Furthermore, let $f_1(x), \ldots, f_N(x)$ be polynomials in x. Then there exists a common domain $\mathcal{D}_L(f) \subset \mathcal{D}$ for the operators of item 1. and of

the operators corresponding to the symols $f_k(q,p) := |f(q)|^2 f_k(q)\, p^{-k}$ with $k = 1,..,N$, 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 reference Thiemann n.d. Thereby, note that $\hat{p}^{-1}$ is a symmetric operator with distribution kernel

$$(\hat{p}^{-1}\psi)(x) = -\frac{i}{2}\int_{\mathbb{R}} \mathrm{d}y\, \mathrm{sgn}(x-y)\psi(y) \tag{7.35}$$

which can easily be seen by applying $\hat{p} = -i\mathrm{d}/\mathrm{d}x$ from the left and using that, $\mathrm{d}\,\mathrm{sgn}(x-y)/\mathrm{d}x = -2\delta(x-y)$ in a distributional sense. The domain of $\hat{p}^{-1}$ must be chosen carefully. Even if ψ is a Schwartz function, while $\hat{p}^{-1}\psi$ is smooth, it may not be of rapid decrease any more at infinity. Likewise, it is a simple corollary that a dense and invariant domain for $\hat{p}^i\hat{q}^j$ with $i \in \mathbb{Z}$, $j \in \mathbb{N}_0$ is given by the Fourier transform of the functions of item 1) but that the Fourier transform is not necessarily of rapid decrease in x any more. This is why the statement of item 3) is significantly weaker, in particular $\mathcal{D}_L(f)$ 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 $\mathcal{D}$ orthogonal to $\mathcal{D}_L(f)$.

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 3) and are finite in number. Thus we use the ordering alluded to in item 3) and the domain described there. The other terms not involving negative powers of p are also defined on that domain since $\mathcal{D}_L(f) \subset \mathcal{D}$.

8. Inhomogeneous Cosmology with Dust

This chapter applies SAPT to a quantum field model which includes a homogeneous and isotropic gravitational field as well as a Klein–Gordon field which is now allowed to be *inhomogeneous*. Besides, we introduce a homogeneous timelike dust field which serves to deparametrize the model in order to have a true Hamiltonian instead of a constraint. This distinguishes this chapter from the following chapter 9 in which we discuss a fully constrained model. In both cases, it is necessary to generalize the standard space adiabatic perturbation approach by Panati, Spohn, and Teufel (2003), because of the henceforward *infinite* number of field degrees of freedom. As before, we are going to split the system into two subsystems where now the inhomogeneous degrees of freedom will be identified with the sector formerly denoted as the fast sector. As such, the model must provide an initial quantum field theoretical model that depends on the homogeneous variables which constitute the remaining part of the system.

One important assumption of SAPT which is trivially satisfied in the quantum mechanical case is that these fast initial quantum problems are mutually unitarily equivalent one to another. This is the statement of the Stone–von Neumann theorem (Neumann 1931, 1932b; Stone 1930, 1932) in quantum mechanics. The Stone–von Neumann theorem does however not apply to quantum *field* theory, and we will use the Hilbert–Schmidt condition (Wald 1995, section 4.4) to explicitely show that the Hilbert spaces of the fast problems are not unitarily equivalent from the outset. As we will see, these problems originating from the infinite number of degrees of freedom can be circumvented using a transformation of the total set of homogeneous and inhomogeneous variables. This transformation is an exact canonical transformation up to second order in the cosmological perturbations. The idea for these transformations orginally comes from the hybrid approach to quantum cosmology as proposed by Castelló Gomar, Martín–Benito, and Mena Marugán (2016), Castelló Gomar, Martín-Benito, and Mena Marugán (2015), and Elizaga Navascués, Martin-Benito, and Mena Marugan (2016).

Accordingly, this chapter starts in section 8.1 with demonstrating the failure of the Hilbert–Schmidt condition for models with an infinite number of degrees of freedom. We subsequently introduce a suitable set of (almost) canonical transformations at the classical level to resolve this issue. This section is based and partly taken from (Schander and Thiemann 2019a). In section 8.2, we apply the scheme to the transformed inhomogeneous Klein–Gordon model with dust. It is based and also partially taken from (Schander and Thiemann 2019b).

8.1. Transformations for Well–Defined Quantum Fields

8.1.1. A Quantum Field Theory with Dust

In this section, we discuss the anomalies that occur in QFT on CST due to the infinite number of degrees of freedom. In particular, it is important to understand how the quantum fields for different configurations of the underlying curved space time can be related one to another. As it turns out, the corresponding natural Fock representations fail to be unitarily equivalent for different configurations of the homogeneous variables. SAPT requires a remedy for this problem due to its tensorial Hilbert space structure.

We illustrate the dilemma with a simple field theoretical model of a classical real–valued scalar field Φ of Klein–Gordon type defined on space time $\mathcal{M} \cong \mathbb{R} \times \sigma$ for which we choose the spatial hypersurface σ to be a flat and compact manifold, i.e., the three–torus $\mathbb{T}^3$. A different choice of topology is possible but since this choice does not affect the essential point of this section, we use the simple three–torus. $\mathcal{M}$ hence foliates into spatial hypersurfaces, each of which has the topology $\mathbb{T}^3$. Therefore, we recall that there exists a diffeomorphism which maps any point $X \in \mathcal{M}$ to its coordinate representative (t, x). The variable x denotes the local coordinates on $\mathbb{T}^3$. The field naturally splits into a purely homogeneous and isotropic part $\phi(t, x) = \phi(t)$ with respect to this hypersurface foliation and we define the difference $\varphi(t, x) := \Phi(t, x) - \phi(t)$ as a linear perturbation of ϕ. Furthermore, the model comprises the homogeneous and isotropic part of the metric field g which has Lorentzian signature $(-, +, +, +)$ as well as a timelike homogeneous and isotropic real scalar dust field u with energy density ρ (J. D. Brown and Kuchar 1995). The homogeneous and isotropic metric reduces to the time–dependent scale factor a, its velocity $\dot{a}$ and the lapse function N. Since N turns out to be a mere Lagrange multiplier (see the Dirac analysis in section 2.1.2), we set $N \equiv 1$. Since we work on compact spatial slices, it is meaningful to isolate the zero mode of the fields and the action splits into a homogeneous and a second order inhomogeneous perturbative part $S = S_{\text{hom}} + S_{\text{pert}}$ with

$$
\begin{aligned}
S_{\text{hom}}[a, u, \phi] &= \int_{\mathbb{R}} \mathrm{d}t \left(-\frac{3a\,\dot{a}^2}{\kappa} + \frac{a^3\,\rho}{2}\left(\dot{u}^2 - 1\right) + \frac{a^3}{2\lambda}\left(\dot{\phi}^2 - m^2\phi^2\right)\right), \\
S_{\text{pert}}[a, \varphi] &= \frac{1}{2\lambda}\int_{\mathbb{R}\times\mathbb{T}^3} \mathrm{d}t\,\mathrm{d}x\, a^3\left(\dot{\varphi}^2 - \frac{(\nabla\varphi)^2}{a^2} - m^2\varphi^2\right)
\end{aligned}
\tag{8.1}
$$

where $\kappa = 8\pi G$ is the gravitational coupling constant, $\lambda \in \mathbb{R}^+$ is the coupling constant of the matter field, $m \in \mathbb{R}^+$ its mass, and we have introduced the measure $\mathrm{d}x$ of the spatial hypersurfaces. The dust field serves to deparametrize the model. Namely, after fixing the gauge freedom associated with the spacetime diffeomorphisms, the gravitational and scalar contribution to the Hamilton constraint combine to build a physical Hamiltonian when integrated over the spatial hypersurface (J. D. Brown and Kuchar 1995; Giesel and Thiemann 2015). The gravitational and the scalar field degrees of freedom become observable fields. Obviously, such a deparametrization simplifies the analysis of the quantum problem significantly but it must be pointed out that this framework does not treat all degrees of freedom at the same level – namely, the dust field is not quantized.

To proceed towards an application of SAPT, we employ a Hamiltonian analysis and perform

a Legendre transformation from which the conjugate momenta (p_a, μ, π) of the scale factor, the homogeneous scalar field and the inhomogeneous part of the scalar field arise in the standard way (cf. section 2.1.2). Together with their conjugate variables (a, ϕ, φ), they constitute the total (now infinite–dimensional) phase space Γ of the system. The transformation yields the Hamilton function $H = H_{\text{hom}} + H_{\text{pert}}$ with

$$H_{\text{pert}}(a, \varphi, \pi) = \frac{1}{2\lambda} \int_{\mathbb{T}^3} \mathrm{d}x \left(\frac{\lambda^2 \pi^2}{a^3} - a\, \varphi(\Delta\varphi) + a^3 m^2 \varphi^2 \right) \tag{8.2}$$

where Δ is the Laplace–Beltrami operator associated with the constant spatial hypersurface $\mathbb{T}^3$. The homogeneous contribution to the Hamiltonian $H_{\text{hom}}(a, p_a, \phi, \mu)$ has the form of the well–known homogeneous and isotropic cosmological Hamilton constraint (7.3) but its explicit form is not important here. SAPT requires to work on a product Hilbert space $\mathcal{H} = \mathcal{H}_{\text{hom}} \otimes \mathcal{H}_{\text{pert}}$ where the first factor refers to the homogeneous sector and the second one to the perturbative sector in our case. This is similar to what we encountered before when splitting into a slow and a fast sector according to $\mathcal{H} = \mathcal{H}_{\text{s}} \otimes \mathcal{H}_{\text{f}}$. As far as the homogeneous sector is concerned, we adopt a usual Schrödinger representation on the Hilbert space $\mathcal{H}_{\text{hom}} = L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}a\, \mathrm{d}\phi)$. Note that this Hilbert space is restricted to the positive half real line in the first factor which requires a proper examination of the operators and their domains defined on it. Regarding the inhomogeneous part, a standard Fock representation suggests itself since $H_{\text{pert}}(a, \varphi, \pi)$ is quadratic in the fields φ and π. But which one? The "background" variable a is not a fixed function of time but a dynamical quantum variable, and hence displays quantum fluctuations. SAPT allows to technically consider the scale factor a as a real parameter at a first stage, namely when quantizing $H_{\text{pert}}(a, \varphi, \pi)$ with respect to the inhomogeneous variables (φ, π). In this case, the system corresponds to a standard quantum Klein–Gordon field with an a–dependent frequency, and the representation will hence depend on the value of a.

To see this, consider the one–particle Hilbert space $\mathcal{H}_{\mathbb{T}^3} := L^2(\mathbb{T}^3, \mathrm{d}x)$ on $\mathbb{T}^3$ and the associated symmetric Fock space $\mathcal{H}_{\text{pert}} = \mathcal{F}_{\text{s}}(\mathcal{H}_{\mathbb{T}^3})$ as the state space of the inhomogeneous quantum field theory. We promote the canonical fields to operator–valued distributions on a suitable space of smearing functions, e.g., the space of smooth functions $C_0^\infty(\mathbb{T}^3)$ with compact support on $\mathbb{T}^3$. The operators will be denoted by bold letters, i.e., $\boldsymbol{\varphi}(f), \boldsymbol{\pi}(f) \in \mathcal{L}(\mathcal{F}_{\text{s}}(\mathcal{H}_{\mathbb{T}^3}))$ with $f \in C_0^\infty(\mathbb{T}^3)$ where $\mathcal{L}$ commonly denotes the space of linear operators. The theory is defined by the commutation relations

$$[\boldsymbol{\varphi}(f_1), \boldsymbol{\pi}(f_2)]_{\text{pert}} = i \langle f_1, f_2 \rangle \mathbf{1}_{\text{pert}} \tag{8.3}$$

where $f_1, f_2 \in C_0^\infty(\mathbb{T}^3)$ are two suitable test functions, $\langle \cdot, \cdot \rangle$ denotes the L^2–scalar product of $L^2(\mathbb{T}^3)$–functions, $\mathbf{1}_{\text{pert}}$ is the one in the corresponding quantum algebra that we denote by $\mathcal{A}_Q$ and we explicitely label the commutator bracket with respect to the perturbative fields with a subscript "pert". In order to define the standard representation in terms of annihilation and creation operators, we introduce the a–dependent one–particle frequency operator $\omega(a)$ according to

$$\omega(a)^2 := -a^4 \Delta + m^2 a^6. \tag{8.4}$$

By duality, this operator can act on the quantum field $\boldsymbol{\varphi}(f) \in \mathcal{L}(\mathcal{F}_{\text{s}}(\mathcal{H}_{\mathbb{T}^3}))$ with $f \in C_0^\infty(\mathbb{T}^3)$ according to $(\sqrt{\omega(a)}(\boldsymbol{\varphi}))(f) := \boldsymbol{\varphi}(\sqrt{\omega(a)}(f))$. A representation $\pi : \mathcal{A}_Q \to \mathcal{L}(\mathcal{F}_{\text{s}}(\mathcal{H}_{\mathbb{T}^3}))$ of the

field algebra in terms of annihilation and creation operators $\boldsymbol{b}$ and $\boldsymbol{b}^*$ can then be defined by

$$\boldsymbol{b}(a,f) := \frac{1}{\sqrt{2}}\pi\left[\left(\sqrt{\omega(a)}\boldsymbol{\phi}\right)(f) - i\left(\sqrt{\omega(a)}^{-1}\boldsymbol{\pi}\right)(f)\right], \tag{8.5}$$

and accordingly for the creation operator with the minus replaced by a plus. Since the representation map depends on the value of a, it makes sense to define $\pi = \pi_a$ with its explicit dependence on a. The commutation relations of the fields become

$$[\boldsymbol{b}(a,f_1),\boldsymbol{b}(a,f_2)]_{\text{pert}} = \langle f_1, f_2\rangle \mathbf{1}_{\text{pert}} \tag{8.6}$$

with $\mathbf{1}_{\text{pert}} \in \mathcal{B}(\mathcal{F}_s(\mathcal{H}_{\mathbb{T}^3}))$. For the following considerations, it is useful to consider an orthonormal basis in $\mathcal{H}_{\mathbb{T}^3}$. Since we are on the three–torus, this basis can be labeled by a discrete set of numbers $k \in \Sigma := 2\pi\mathbb{Z}^3$. We denote this basis by $\{f_k\}_{k\in\Sigma}$ and require the functions f_k to be eigenfunctions of the Laplace–Beltrami operator on $\mathbb{T}^3$ with eigenvalues $-k^2$ respectively. Since we associate the zero mode $k = 0$ with the homogeneous mode of the scalar field, it will be excluded in the following considerations regarding the purely inhomogeneous field theory. We define $\Bbbk := 2\pi\mathbb{Z}^3 \setminus \{0\}$. Hence, the frequency operator $\omega(a)$ for every $a \in \mathbb{R}^+$ acts on some f_k with $k \in \Bbbk$ according to

$$\omega(a)f_k = \sqrt{a^4k^2 + m^2a^6}f_k =: \omega(a,k^2)f_k. \tag{8.7}$$

On the normalized three–torus, the basis functions can be given more explicitely by the plane waves $f_k(x) = \exp(ikx)$, $x \in \mathbb{T}^3$. It is convenient to introduce the annihilation and creation operators for the modes f_k, which satisfy the standard commutation relations of annihilation and creation operators, namely

$$[\boldsymbol{b}(a,f_k),\boldsymbol{b}^*(a,f_{k'})]_{\text{pert}} = \delta_{k,k'}\mathbf{1}_{\text{pert}}, \quad \forall a \in \mathbb{R}^+ \tag{8.8}$$

where $\delta_{k,k'}$ is the Kronecker delta with respect to the discrete modes k and k'. A representation of the quantization $\boldsymbol{H}_{\text{pert}}$ of the perturbative Hamiltonian in terms of these mode annihilation and creation operators gives the model the form of a discrete but infinite set of independent harmonic oscillators with respective frequencies $\omega(a,k^2)$. A normal ordering of the Fock–quantized perturbation Hamiltonian $\boldsymbol{H}_{\text{pert}}$ yields

$$\boldsymbol{H}_{\text{pert}}(a) = \frac{1}{a^3}\sum_{k\in\Bbbk}\boldsymbol{b}^*(a,f_k)(\omega(a)\,\boldsymbol{b}(a))(f_k). \tag{8.9}$$

This expression has the standard form of a Hamilton operator in quantum field theory on Minkowski space time – with the difference that the frequency as well as the annihilation and creation operators depend on the scale factor. The question is how the natural basis states induced by the annihilation operators are related for different values of a.

8.1.2. Violation of the Hilbert–Schmidt Condition

The question of the relation between the different representations π_a and of how the natural states induced by these representations are linked can be formulated in the following way:

1. Are the a–dependent Fock representations $(\pi_a, \mathcal{F}_s)$ with the group homomorphisms $\pi_a : \mathcal{A}_Q \to \mathcal{L}(\mathcal{F}_s)$ that map the field Weyl algebra associated with $(\boldsymbol{\varphi}, \boldsymbol{\pi})$ to the space of bounded linear operators on $\mathcal{F}_s$ all unitarily equivalent to a single representation $(\pi_0, \mathcal{F}_s)$? This is one of the innocent looking assumptions of SAPT in quantum mechanics.

2. Assuming that this unitary equivalence between the different representations is granted, let f be a smooth function in $\mathcal{H}_{\mathbb{T}^3}$ and $\hat{\boldsymbol{b}}(a, f) := \hat{\mathcal{W}}(\boldsymbol{b}(a, f))$ and $\widehat{\boldsymbol{b}^*}(a, f) := \hat{\mathcal{W}}(\boldsymbol{b}^*(a, f))$ the Weyl quantizations of $\boldsymbol{b}(a, f)$ and $\boldsymbol{b}^*(a, f)$ with respect to the homogeneous variables, i.e., with respect to the scale factor here. Then, is the complete algebra of operators $\hat{a}$, $\hat{p}_a$, $\hat{\phi}$, $\hat{\mu}$, $\hat{\boldsymbol{b}}(a, f)$, $\widehat{\boldsymbol{b}^*}(a, f)$ well–defined on the full Hilbert space $\mathcal{H}_{\text{hom}} \otimes \mathcal{H}_{\text{pert}}$?

It turns out that both questions are tightly related and that the answer to both is in the negative. The underlying effect has been first observed by Castelló Gomar, Martín–Benito, and Mena Marugán (2016), Castelló Gomar, Martín-Benito, and Mena Marugán (2015), and Elizaga Navascués, Martin-Benito, and Mena Marugan (2016) 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 natural Fock vacuum $\Omega(a_2)$ associated with the representation π_{a_2} can be written as a (possibly excited) state with respect to states associated with the representation π_{a_1} for all distinct a_1, a_2 in $\mathbb{R}^+$. In fact, this condition is also sufficient because polynomials of the creation operators $\boldsymbol{b}^*(a_1, f)$ can then be written as polynomials of the operators $\boldsymbol{b}(a_2, f)$ and $\boldsymbol{b}^*(a_2, f)$ for some smooth $f \in C_0^\infty(\mathbb{T}^3)$.

Relation of Vacua

To elaborate on this, let (n) denote the collection of occupation numbers $\{n_k\}_{k\in\mathbb{k}}$ of some excited state $\psi_{(n)}$ within the π_{a_1}–representation. We define this excited state in the standard manner as

$$\psi_{(n)}(a_1) = \prod_{k\in\mathbb{k}} \frac{[\boldsymbol{b}^*(a_1, f_k)]^{n_k}}{\sqrt{n_k!}}\, \Omega(a_1) \tag{8.10}$$

where $\Omega(a_1)$ is the standard vacuum state associated with the representation π_{a_1}, i.e., it satisfies $\boldsymbol{b}(a_1, f_k)\Omega(a_1) = 0$ for all $k \in \mathbb{k}$. We then assume that it is possible to write the natural vacuum state associated with π_{a_2} as a linear combination of such excited states, namely

$$\Omega(a_2) = \sum_{(n)} z_{(n)} \cdot \psi_{(n)}(a_1) \tag{8.11}$$

where the sum is over all (n) with only finitely many n_k different from zero. We then require that $\boldsymbol{b}(a_2, f_k)\,\Omega(a_2) = 0$ is satisfied for any $k \in \mathbb{k}$. To analyze this equation with respect to the π_{a_1}–representation, consider the one–particle operators $u_\pm(a_1, a_2) : C_0^\infty(\mathbb{T}^3) \to C_0^\infty(\mathbb{T}^3)$ defined by

$$u_\pm(a_1, a_2) := \frac{1}{2}\left(\sqrt{\frac{\omega(a_1)}{\omega(a_2)}} \pm \sqrt{\frac{\omega(a_2)}{\omega(a_1)}}\right), \tag{8.12}$$

and we recall that these correspond to the Bogoliubov coefficients already encountered in section 4.1. By extending $u_\pm(a_1, a_2)$ to the space of operator–valued distributions as before, we define the

Bogoliubov transformation by

$$\boldsymbol{b}(a_2, f_k) := (u_+(a_1, a_2)\,\boldsymbol{b}(a_1))(f_k) + (u_-(a_1, a_2)\,\boldsymbol{b}^*(a_1))(f_k) \tag{8.13}$$

for any $f_k \in C_0^\infty(\mathbb{T}^3)$ and linear combinations thereof. The one–particle operator $u_\pm(a_1, a_2)$ is diagonal with respect to the basis states $\{f_k\}_{k\in\Bbbk}$. Therefore, let $u_\pm(a_1, a_2, k^2) \in \mathbb{R}$ be the eigenvalues of $u_\pm(a_1, a_2)$ defined by $u_\pm(a_1, a_2)\, f_k = u_\pm(a_1, a_2, k^2)\, f_k$. It follows by extending this relation to the operator–valued distributions that

$$(u_+(a_1, a_2)\,\boldsymbol{b}(a_1))(f_k) = u_+(a_1, a_2, k^2)\,\boldsymbol{b}(a_1, f_k) \tag{8.14}$$

and correspondingly for $u_-(a_1, a_2)$ and $\boldsymbol{b}^*(a_1, f_k)$. Eventually, let us introduce the following notation: We denote the collection of occupation numbers for which only the excitation number associated with f_k equals one and the remaining ones all vanish by 1_k. Then, the expression $(n)\pm 1_k$ stands for a set of occupation numbers in which the excitation number of f_k in the set (n) is raised or lowered respectively by one. Then, we require that the defining equation of the vacuum state holds, namely that the application of the annihilation operator $\boldsymbol{b}(a_2, f_k)$ on the vacuum state $\Omega(a_2)$ vanishes independently for all $k \in \Bbbk$ and get

$$\begin{aligned}
&\boldsymbol{b}(a_2, f_k)\Omega(a_2) \qquad\qquad (8.15)\\
&\quad= \sum_{(n)} z_{(n)}\Big[\sqrt{n_k}\, u_+(a_1, a_2, k^2)\, \psi_{(n)-1_k}(a_1) + \sqrt{n_k+1}\, u_-(a_1, a_2, k^2)\, \psi_{(n)+1_k}(a_1)\Big]\\
&\quad= \sum_{(n)} \Big[z_{(n)+1_k}\, u_+(a_1, a_2, k^2)\sqrt{n_k+1} + z_{(n)-1_k}\, u_-(a_1, a_2, k^2)\sqrt{n_k}\Big]\, \psi_{(n)}(a_1) \stackrel{!}{=} 0.
\end{aligned}$$

Since the relation (8.15) holds for all $k \in \Bbbk$ independently, the coefficients must be of infinite product type, i.e., of the form

$$z_{(n)} = \prod_k \zeta^k_{n_k}. \tag{8.16}$$

Then, we define the quotient $\theta(a_1, a_2, k^2) := u_-(a_1, a_2, k^2)/u_+(a_1, a_2, k^2)$. The product ansatz together with this definition transforms equation (8.15) into the recursion relation,

$$\zeta^k_{n_k+1} = -\sqrt{\frac{n_k}{n_k+1}}\,\theta(a_1, a_2, k^2)\, \zeta^k_{n_k-1}. \tag{8.17}$$

The right hand side of the recursion relation vanishes for $n_k = 0$. It follows that $\zeta^{n_k}_{(n)} = 0$ for any odd n_k. For n_k even, the solution of equation (8.17) is given by

$$\zeta^k_{2n_k} = -\sqrt{\frac{2n_k-1}{2n_k}}\,\theta(a_1, a_2, k^2)\, \zeta^k_{2(n_{k-1})} = (-\theta(a_1, a_2, k^2))^{n_k}\sqrt{\frac{(2n_k)!}{4^{n_k}(n_k!)^2}}\,\zeta^k_0 \tag{8.18}$$

where for the time being, the ζ^k_0 remain undetermined and their values are of no relevance for the subsequent argumentation. In order to prove that the vacuum $\Omega(a_1)$ transforms into the vacuum $\Omega(a_2)$ in a well–defined fashion, it is necessary that the $\mathcal{F}_s$–norm of $\Omega(a_2)$ within the π_{a_1}–representation has a finite non–vanishing value. As a working hypothesis, we assume that this is

true. Then, it stems from the previous results that

$$\begin{aligned}\|\Omega(a_2)\|^2_{\mathcal{F}_s} &= \sum_{(n)} |z_{(n)}|^2 = \sum_{(n)} \Big| \prod_{k\in\mathbb{k}} \zeta^k_{n_k} \Big|^2 = \sum_{(n)} \prod_{k\in\mathbb{k}} \Big|\zeta^k_{n_k}\Big|^2 \\ &= \prod_{k\in\mathbb{k}} \left(\sum_{n=0}^{\infty} \Big|\zeta^k_0\Big|^2 \theta(a_1,a_2,k^2)^{2n} \frac{(2n)!}{4^n (n!)^2} \right) \\ &= \Big(\prod_{k\in\mathbb{k}} \Big|\zeta^k_0\Big|^2 \Big) \cdot \Big(\prod_{k\in\mathbb{k}} \sum_{n=0}^{\infty} \theta(a_1,a_2,k^2)^{2n} \frac{(2n)!}{4^n (n!)^2} \Big). \end{aligned} \tag{8.19}$$

Regarding the n–dependent factors in the last expression, it holds true that

$$\frac{1}{2^n} \;\leq\; \frac{(2n)!}{4^n (n!)^2} \;\leq\; 1 \tag{8.20}$$

using mathematical induction. Inserting the estimate (8.20) into (8.19) allows to rewrite the sum as a geometric series. Namely, we then obtain products of infinite series over n with coefficients $(\theta(a_1,a_2,k^2)^{2n})/2^n$ and $\theta(a_1,a_2,k^2)^{2n}$ respectively. Since $\theta(a_1,a_2,k^2)^2 < 1$ independently of k^2, this gives rise to the following estimate:

$$\prod_{k\in\mathbb{k}} \Big|\zeta^k_0\Big|^2 \cdot \prod_{k\in\mathbb{k}} \left(1 - \frac{\theta(k^2)^2}{2}\right)^{-1} \leq \|\Omega(a_2)\|^2_{\mathcal{F}_s(a_1)} \leq \prod_{k\in\mathbb{k}} \Big|\zeta^k_0\Big|^2 \cdot \prod_{k\in\mathbb{k}} \big(1 - \theta(k^2)^2\big)^{-1}.$$

Thus, a necessary condition for the convergence of (8.19) is that the two infinite products converge independently to a finite non–zero value. Note thereby that $\prod_{k\in\mathbb{k}} |\zeta^k_0|^2$ is a common prefactor in all $|z_{(n)}|^2$, and thus must converge to some finite value as otherwise the $z_{(n)}$ would be meaningless. By taking the logarithm, the convergence of the lower estimate is equivalent to the convergence of the series

$$\sum_{k\in\mathbb{k}} \ln\left(1 - \frac{\theta(a_1,a_2,k^2)^2}{2}\right) \tag{8.21}$$

which is also known as the *Hilbert–Schmidt condition* (Wald 1995). In order to resolve the estimates, we recall that $\theta(a_1,a_2,k^2)$ is determined by the frequency function $\omega(a,k^2)$, namely

$$\theta(a_1,a_2,k^2)^2 = \frac{u_-(a_1,a_2,k^2)^2}{u_+(a_1,a_2,k^2)^2} = \frac{((a_1^4 - a_2^4)k^2 + (a_1^6 - a_2^6)m^2)^2}{(\omega(a_1,k^2) + \omega(a_2,k^2))^4}. \tag{8.22}$$

A necessary condition for the series (8.21) to converge is that the coefficients of the latter tend to zero for $k^2 \to \infty$. Keeping track of the logarithm, this is true if $\theta(a_1,a_2,k^2)^2$ tends to zero. To check this, note that $\omega(a,k^2) \to a^2|k|$ for large k^2. Consequently, expression (8.21) evaluates to

$$\lim_{k\to\infty} \theta(a_1,a_2,k^2)^2 = \frac{(a_1^2 - a_2^2)^2}{(a_1^2 + a_2^2)^2} \tag{8.23}$$

which is a non–vanishing constant for $a_1 \neq a_2$ and consequently, the Hilbert–Schmidt condition fails for any two distinct a_1, a_2. Note however that according to equation (8.22), the problem would disappear if the wave mode term was relieved from its scale factor dependence. In particular, then $\theta(a_1,a_2,k^2)^2$ would decay like $1/k^4$, and thus the series $\sum_k \ln(1 - \theta(a_1,a_2,k^2)^2)$ would converge to a non zero value. This answers the first question posed above, namely that the Fock

representations $(\pi_a, \mathcal{F}_s)$ are *not* unitarily equivalent for different values of a, except in the case that the contribution carrying the Laplace–Beltrami operator in the one–particle frequency operator $\omega(a, k^2)$ is independent of the scale factor, or more generically, independent of the homogeneous phase space variables.

Definition of the Operator Algebra

The second question, i.e., whether the complete operator algebra of the canonical pairs is well defined on the full Hilbert space, is in fact equivalent to the first one. To see this, we assume that the scale factor a is represented as a self–adjoint operator $\hat{a}$ on a dense domain of the full Hilbert space $\mathcal{H}$. The spectral theorem then allows to display the Hilbert space as a direct integral or a Hilbert bundle subordinate to a according to

$$\mathcal{H} \cong \int_{\sigma(\hat{a})}^{\oplus} \mathrm{d}\mu(a)\, \mathcal{H}_{\mathrm{pert}}(a) \tag{8.24}$$

where μ is the spectral probability measure on the spectrum $\sigma(\hat{a})$ of $\hat{a}$ which is just $\mathbb{R}_0^+$. The previous discussion suggests to identify the fibre spaces $\mathcal{H}_{\mathrm{pert}}(a)$ with the Fock space $\mathcal{F}_s$ with different a–dependent vacua. As a consequence of the spectral theorem, the Hilbert spaces $\mathcal{F}_s$ must be chosen identical (Reed and Simon 1975a,b) but this is not possible according to the former considerations.

Let us assume the opposite for the time being. Then, vectors in the Hilbert bundle are given by measurable fibre Hilbert space valued functions $\psi : \sigma(\hat{a}) \mapsto \mathcal{H},\ a \mapsto \psi(a)$ over the base manifold $\sigma(\hat{a})$. They are equipped with the inner product

$$\langle \psi, \psi' \rangle_{\mathcal{H}} = \int_{\sigma(\hat{a})} \mathrm{d}\mu(a) \langle \psi(a), \psi'(a) \rangle_{\mathcal{F}_s}. \tag{8.25}$$

By the spectral theorem, $\hat{a}$ acts by multiplication in the fibre $\mathcal{F}_s$. Accordingly, the operator $\hat{\boldsymbol{H}}_{\mathrm{pert}}$ acts fibre wise by the symbol $\boldsymbol{H}_{\mathrm{pert}}(a)$ in equation (8.9). The question is how the operator $\hat{p}_a$ representing the momentum conjugate to the scale factor acts on the direct integral Hilbert space. As the spectrum of $\hat{a}$ is of the absolutely continuous type, the momentum acts as $(\hat{p}_a \psi)(a) = (i\partial_a + f(a))\, \psi(a)$ where we introduce the function $f(a)$ related to the divergence of the measure $\mu(a)$. The function has the purpose to turn $\hat{p}_a$ into a symmetric operator. In fact, in order to obtain a self–adjoint operator, it is advisable to pass to the real–valued triad variable b (like in the previous chapter) and work with its conjugate momentum. Nevertheless, the conclusion derived below is not affected by these subtleties.

In order to check whether the geometric momentum operator $\hat{p}_a$ is well–defined on (some dense subset of) $\mathcal{H}$, we compute the norm of the state $(\hat{p}_a\, \Omega)(a)$. Therefore, consider the geometric commutator of $\hat{p}_a$ and $\hat{\boldsymbol{b}}(a, f)$ in an integral representation. As the operator $\boldsymbol{b}(a, f)$ only depends on the configuration variable a, a partial integration allows to shift the derivative due to $\hat{p}_a$ on $\boldsymbol{b}(a, f)$. Using equation (8.5), we see that the derivative directly acts on powers of the one–particle operator $\omega(a)$ within $\boldsymbol{b}(a, f)$. This yields an a–dependent one–particle operator $K(a)$

subject to the geometric quantization procedure

$$\left[\, \hat{p}_a, \hat{\boldsymbol{b}}(a,f) \,\right] = -i(\hat{K}(a)\,\widehat{\boldsymbol{b}^*}(a))(f) \quad \text{where } K(a) := \frac{1}{2}\frac{\partial_a \omega(a)}{\omega(a)} \tag{8.26}$$

and where for notational convenience the hats indicating the Weyl quantization with respect to the homogeneous variables rather sit on the operator labels than on their arguments. As a result of equation (8.26) and with the requirement $\hat{\boldsymbol{b}}(a,f)\,\Omega(a) = 0$ for any $f \in C_0^\infty(\mathbb{T}^3)$, it holds true that

$$\hat{\boldsymbol{b}}(a,f)\,(\hat{p}_a\Omega) = \left[\hat{\boldsymbol{b}}(a,f), \hat{p}_a\right]\,\Omega = i\,(\hat{K}(a)\,\widehat{\boldsymbol{b}^*}(a))(f)\,\Omega. \tag{8.27}$$

Using that any one–particle state f has a unique decomposition with respect to some basis $\{f_k\}_{k\in\mathbb{k}}$ and that the above equality must hold for *any* f, the vector $\hat{p}_a\Omega$ is given by

$$\hat{p}_a\Omega = -\frac{i}{2}\sum_{k\in\mathbb{k}} \widehat{\boldsymbol{b}^*}(a,f_k)\,(\hat{K}(a)\,\widehat{\boldsymbol{b}^*}(a))(f_k)\,\Omega. \tag{8.28}$$

This allows us to compute the norm of $\hat{p}_a\Omega$. Therefore, we denote the twofold excitation of the vacuum state $\Omega(a)$ with respect to the mode f_k by $\sqrt{2}\,\psi_{2_k}(a)$. Then, using the inner product with respect to the geometric quantization, we obtain for the norm squared

$$\begin{aligned} \|\,\hat{p}_a\Omega\|^2_{\mathcal{F}_s} &= \int_{\sigma(\hat{a})} \mathrm{d}\mu(a) \sum_{k\in\mathbb{k}} \langle \psi_{2_k}(a)\,K(a,k^2), K(a,k^2)\,\psi_{2_k}(a)\rangle_{\mathcal{F}_s} \\ &= \frac{1}{16}\int_{\sigma(\hat{a})} \mathrm{d}\mu(a) \sum_{k\in\mathbb{k}} \left(\frac{\partial_a\omega(a,k^2)^2}{\omega(a,k^2)^2}\right)^2 . \end{aligned} \tag{8.29}$$

The norm only admits a finite value if the sum over k is almost everywhere finite as a function of a. However, for large k any coefficient of the series evaluates to $(4/a)^2$ which is a constant for some fixed value of the scale factor a. Hence, the sum does not converge and $\hat{p}_a\Omega$ has infinite norm. Note that equation (8.29) is the infinitesimal version of equation (8.21) which becomes clear by dividing the latter by $(a_1 - a_2)^2$ and taking the limit $a_2 \to a_1$. Consequently, SAPT cannot be applied to QFT on CST without further ado.

8.1.3. A Simple Transformation

One hope might be that with a different choice of Fock representations the Hilbert–Schmidt condition can be met for example by a simple canonical rescaling of the field operators. However, if the correspondingly normal–ordered Hamiltonian should remain at least densely defined on the Fock states, this again leads to an obstruction. To understand the origin of this impediment, note that we can satisfy the Hilbert–Schmidt condition by rescaling the classical (distributional) fields $\varphi(f)$ and $\pi(f)$ according to

$$\tilde{\varphi}(f) := a\,\varphi(f), \qquad \tilde{\pi}(f) := \frac{\pi(f)}{a}. \tag{8.30}$$

The new fields still satisfy the canonical Poisson brackets with respect to the *inhomogeneous* degrees of freedom if a is held fixed, i.e., $\{\tilde{\varphi}(f_1), \tilde{\pi}(f_2)\}_{\text{pert}} = \langle f_1, f_2\rangle$ for any $f_1,\, f_2 \in C_0^\infty(\mathbb{T}^3)$,

and we recall that $\langle\cdot,\cdot\rangle$ is the scalar product in $L^2(\mathbb{T}^3)$. The perturbative Hamilton function then becomes

$$H_{\text{pert}}(a) = \frac{1}{2a}\int_{\mathbb{T}^3} \mathrm{d}x\left(\tilde{\pi}^2 + \tilde{\varphi}\,\tilde{\omega}(a)\tilde{\varphi}\right) \quad \text{where} \quad \tilde{\omega}(a) = -\Delta + m^2a^2. \tag{8.31}$$

Note that now the coefficient of the Laplace operator in $\tilde{\omega}(a)^2$ is *independent* of a. However, the transformation (8.30) is not a canonical transformation on the *full* phase space. In fact, it is no longer the case that p_a, $\tilde{\varphi}$ and $\tilde{\pi}$ have vanishing Poisson brackets as the above transformation depends on a. Consequently, the fundamental canonical structure is lost. However, the transformation (8.30) allows for an *exact* completion by adding a corresponding contact term in the symplectic potential.

To define the symplectic potential for the system, we recall that it is modelled on an infinite dimensional Banach manifold $\mathcal{C}$ which is given by the Cartesian product of the finite dimensional, homogeneous configuration space $\mathcal{C}_{\text{hom}} = \mathbb{R}^+\times\mathbb{R}$ and the infinite dimensional, perturbative configuration space of fields $\mathcal{C}_{\text{pert}}$. The latter space could for example be the Sobolev space $H^1(\mathbb{T}^3)$ of fields whose first derivatives have a finite L^2–norm such that the Hamilton function is well defined. With the cotangent bundle $T^*\mathcal{C}$ (i.e., the phase space associated with $\mathcal{C}$) and the projection map $\mathrm{pr} : T^*\mathcal{C} \to \mathcal{C}$, we define the symplectic potential Θ on the manifold $T^*\mathcal{C}$ as a map from the tangent space $T_\alpha(T^*\mathcal{C})$ into $\mathbb{R}$ where $\alpha \in T^*_q\mathcal{C}$ with $q = \mathrm{pr}(\alpha)$. In particular, for some $v \in T_\alpha(T^*\mathcal{C})$, we have that $\Theta(\alpha)(v) := \alpha(\mathrm{pr}^*(v))$ where $\mathrm{pr}^* : T(T^*\mathcal{C}) \to T\mathcal{C}$ is the pushforward of the projection pr (Chernoff and Marsden 1974).

In a coordinate representation, this has the standard intuitive form: We denote the coordinates of a point $(q,p) \in T^*_\Phi\mathcal{C}$ in phase space by (Φ,Π) where Φ stands for the generalized fields (a,ϕ,φ). Then, Θ has the coordinate representation $\int_{\mathcal{C}} \mathrm{d}x\,\Pi(x)\mathrm{d}\Phi(x)$ where d is the exterior derivative such that $\mathrm{d}\Phi(x)$ denotes a standard one–form on $T_{(\Phi,\Pi)}(T^*\mathcal{C})$ (Cartan 1970). To shorten the notation, we simply denote the integral by $\langle\Pi,\mathrm{d}\Phi\rangle$. By splitting the fields into the homogeneous and inhomogeneous components and by executing the integrals over the homogeneous degrees of freedom, we obtain

$$\Theta = p_a\mathrm{d}a + \mu\,\mathrm{d}\phi + \langle\pi,\mathrm{d}\varphi\rangle \tag{8.32}$$

where we used the product rule for the exterior derivative. The transformation leading to the dashed fields produces an additional term in the transformed symplectic potential which is then given by

$$\Theta = \left(p_a - \frac{1}{a}\langle\pi,\varphi\rangle\right)\mathrm{d}a + \mu\,\mathrm{d}\phi + \langle\tilde{\pi},\mathrm{d}\tilde{\varphi}\rangle. \tag{8.33}$$

This suggests to define new dashed pairs of conjugate variables for the homogeneous sector, namely

$$\tilde{p}_a := p_a - \frac{1}{a}\langle\pi,\varphi\rangle = p_a - \frac{1}{a}\langle\tilde{\pi},\tilde{\varphi}\rangle, \quad \tilde{a} := a, \quad \tilde{\phi} := \phi, \quad \tilde{\mu} := \mu \tag{8.34}$$

which would complete the transformation. Unfortunately, now we have to write the homogeneous Hamiltonian H_{hom} in terms of $\tilde{p}_a$ and this causes problems when passing to the quantum realm. In particular, when quantizing with respect to the perturbative Fock fields as suggested by SAPT, the supplementary term due to the completion introduces first and second powers of an ill–defined (normal ordered) operator. By taking an arbitrary basis $\{f_k\}_{k\in\mathbb{k}}$ of $L^2(\mathbb{T}^3)$, this operator

is given by

$$\sum_{k\in\mathbb{k}} \tilde{\boldsymbol{\pi}}(f_k)\tilde{\boldsymbol{\varphi}}(f_k) = \frac{i}{2}\sum_{k\in\mathbb{k}} \left(\tilde{\boldsymbol{b}}(a,f_k)^2 - \tilde{\boldsymbol{b}}^*(a,f_k)^2 - 2\,\tilde{\boldsymbol{b}}^*(a,f_k)\,\tilde{\boldsymbol{b}}(a,f_k)\right) \tag{8.35}$$

where $\tilde{\boldsymbol{b}}$ is the annihilation operator obtained from (8.5) by substituting all ingredients by those with a tilde and likewise for the creation operator $\tilde{\boldsymbol{b}}^*$. The operator (8.35) is obviously ill–defined on the corresponding Fock space.

8.1.4. General Class of Transformations

Eventually, this discussion suggests to consider more general transformations in order to avoid the desastrous terms such as (8.35). To determine the class of admissible transformations, we follow the procedure introduced by Castelló Gomar, Martín–Benito, and Mena Marugán 2016; Castelló Gomar, Martín-Benito, and Mena Marugán 2015; Elizaga Navascués, Martin-Benito, and Mena Marugan 2016. Their considerations restrict to perturbation theory up to second order in the fields φ and π which themselves are considered to be of first order. This advocates to confine to transformations linear in φ and π such as (8.30), keeping the second order nature of H_{pert} while higher order transformations would not be visible at the second order precision of H_{pert}. The corresponding contact terms for the homogeneous degrees of freedom will then be of second order at leading order as in equation (8.34).

To shorten the notation, we use the letters (q,p) for collectively denoting the homogeneous variables (a,p_a) and (ϕ,μ). Whenever a distinction is necessary we label them by indices (q^j,p_j) with $j=1,2$. We consider the classical fields $(\varphi,\pi)\in H^3(\mathbb{T}^3)\times H^2(\mathbb{T}^3)$ and apply a set of transformations, (r,s,t,u) which relate the original fields (φ,π) and the transformed fields $(\tilde{\varphi},\tilde{\pi})$. Note that these transformations are operators on the space of (a certain class of) functions, or rather fields, on $\mathbb{T}^3$. We define them by

$$\varphi(f) := (r(q,p)\,\tilde{\varphi}(q,p))(f) + (s(q,p)\,\tilde{\pi}(q,p))(f), \tag{8.36}$$

$$\pi(f) := (t(q,p)\,\tilde{\varphi}(q,p))(f) + (u(q,p)\,\tilde{\pi}(q,p))(f) \tag{8.37}$$

for a smearing field f. We keep the transformations (r,s,t,u) as generic as possible and let them depend on all homogeneous degrees of freedom (q,p). Furthermore, they may involve the Laplace–Beltrami operator which consequently yields non–trivial but translation invariant operators on the field space.

Regarding the Hilbert–Schmidt condition, it suffices to restrict the transformations to depend on the Laplacian so that they mutually commute and are symmetric on $L^2(\mathbb{T}^3)$. Of course, r,s,t and u are restricted to be real–valued since all the variables are. The following analysis shows that the transformations must meet certain conditions. The first requirement results from conditions on the Poisson brackets of the transformed fields. In particular, the new system of fields should satisfy the standard Poisson bracket relations with respect to the inhomogeneous fields such that the transformations (8.36) and (8.37) be canonical. With the two smearing functions

$f_1, f_2 \in C_0^\infty(\mathbb{T}^3)$ we require that

$$\{\varphi(f_1), \pi(f_2)\} = \langle f_1, f_2\rangle = \{\tilde{\varphi}(f_1), \tilde{\pi}(f_2)\}. \tag{8.38}$$

By shifting the transformation operators r, s, t and u on the smearing fields f_1 and f_2, it must hence hold true that

$$\langle(-t\,s + u\,r)\,f_1, f_2\rangle = \langle f_1, f_2\rangle \quad \Rightarrow \quad u\,r - s\,t = 1. \tag{8.39}$$

We emphasize that the symmetry of the respective kernels was exploited and that $([r,s])(f) = ([t,u])(f) = 0$ due to mutual commutativity of the operators. Further conditions for the operators (r,s,t,u) arise from plugging the transformations (8.36) and (8.37) into the symplectic potential (8.32). This generates terms in the symplectic potential giving rise to transformations of the homogeneous variables at second order in the perturbations. When plugging this whole new set of transformed variables into the Hamiltonian and expanding up to second order in the perturbations, new terms in the Hamiltonian emerge. The fact that some of these terms would engender operators in the quantum theory that are not well defined on the Fock space allows to confine the possible transformations (r,s,t,u). It is even possible to restrict the transformations in such a way that all the Fock spaces $\mathcal{F}_\mathrm{s}$ become identical. The condition for this is that the Laplace–Beltrami operator in the effective frequency of the Klein–Gordon field remains independent of the homogeneous phase space variables. The symplectic potential is given by

$$\begin{aligned}\Theta &= p_j\,\mathrm{d}q^j + \langle\pi, \mathrm{d}\varphi\rangle = p_j\,\mathrm{d}q^j + \langle(t\,\tilde{\varphi}) + (u\,\tilde{\pi}), \mathrm{d}((r\,\tilde{\varphi}) + (s\,\tilde{\pi}))\rangle \\ &= p_j\,\mathrm{d}q^j + \langle\tilde{\pi}\,(u\,r - t\,s), \mathrm{d}\tilde{\varphi}\rangle - \frac{1}{2}\left(\langle\tilde{\varphi}, \mathrm{d}(t\,r)\,\tilde{\varphi}\rangle + \langle\tilde{\pi}, \mathrm{d}\,(u\,s)\,\tilde{\pi}\rangle + 2\langle\tilde{\varphi}, \mathrm{d}\,(t\,s)\,\tilde{\pi}\rangle\right) \\ &\quad + \langle\tilde{\varphi}, (t\,\mathrm{d}r)\,\tilde{\varphi}\rangle + \langle\tilde{\varphi}, (t\,\mathrm{d}s + u\,\mathrm{d}r)\,\tilde{\pi}\rangle + \langle\tilde{\pi}, (u\,\mathrm{d}s)\tilde{\pi}\rangle\end{aligned} \tag{8.40}$$

where the second equality was obtained by using that $\langle t\tilde{\varphi}, r(\mathrm{d}\varphi)\rangle = -\langle\mathrm{d}(r\,t\,\tilde{\varphi}), \tilde{\varphi}\rangle$. By means of the product rule for the exterior derivative, we let "d" act on $(r\,t)$ and on $\tilde{\varphi}$. This gives, $-\langle\tilde{\varphi}, \mathrm{d}(r\,t)\tilde{\varphi}\rangle - \langle r\,t\,\tilde{\varphi}, \mathrm{d}\tilde{\varphi}\rangle$. We recognize that the last term corresponds to the original term with a minus sign and by shifting the expressions, we obtain that $\langle t\tilde{\varphi}, r(\mathrm{d}\varphi)\rangle$ equals $-(1/2)\langle\tilde{\varphi}, \mathrm{d}(r\,t)\tilde{\varphi}\rangle$. This method yields all the terms with a factor $(1/2)$ in the second line. Since the operators depend on the homogeneous variables (q, p), we further obtain

$$\begin{aligned}\Theta &= p_j\,\mathrm{d}q^j + \langle\tilde{\pi}, \mathrm{d}\tilde{\varphi}\rangle - \frac{1}{2}\left(\langle\tilde{\varphi}, \partial_{q^j}(t\,r)\,\tilde{\varphi}\rangle + \langle\tilde{\pi}, \partial_{q^j}(u\,s)\,\tilde{\pi}\rangle + 2\langle\tilde{\varphi}, \partial_{q^j}(t\,s)\,\tilde{\pi}\rangle\right)\mathrm{d}q^j \\ &\quad - \frac{1}{2}\left(\langle\tilde{\varphi}, \partial_{p_j}(t\,r)\,\tilde{\varphi}\rangle + \langle\tilde{\pi}, \partial_{p_j}(u\,s)\,\tilde{\pi}\rangle + 2\langle\tilde{\varphi}, \partial_{p_j}(t\,s)\,\tilde{\pi}\rangle\right)\mathrm{d}p_j \\ &\quad + \left(\langle\tilde{\varphi}, t\,(\partial_{q^j}r)\,\tilde{\varphi}\rangle + \langle\tilde{\phi}, (t\,(\partial_{q^j}s) + u\,(\partial_{q^j}r))\,\tilde{\pi}\rangle + \langle\tilde{\pi}, u\,(\partial_{q^j}s)\,\tilde{\pi}\rangle\right)\mathrm{d}q^j \\ &\quad + \left(\langle\tilde{\varphi}, t\,(\partial_{p_j}r)\,\tilde{\varphi}\rangle + \langle\tilde{\varphi}, (t\,(\partial_{p_j}s) + u\,(\partial_{p_j}r))\,\tilde{\pi}\rangle + \langle\tilde{\pi}, u\,(\partial_{p_j}s)\,\tilde{\pi}\rangle\right)\mathrm{d}p_j.\end{aligned} \tag{8.41}$$

In a final step, let us shift the differential in $\mathrm{d}p_j$ to its prefactor using that total differentials vanish

such that

$$\begin{aligned}\Theta = &\langle\tilde{\pi}, \mathrm{d}\tilde{\varphi}\rangle \\ &+ \Big[p_j - \frac{1}{2}\left(\langle\tilde{\varphi}, \partial_{q^j}(t\,r)\,\tilde{\varphi}\rangle + \langle\tilde{\pi}, \partial_{q^j}(u\,s)\,\tilde{\pi}\rangle + 2\langle\tilde{\varphi}, \partial_{q^j}(t\,s)\,\tilde{\pi}\rangle\right) \\ &\quad + \langle\tilde{\varphi}, t\,(\partial_{q^j} r)\,\tilde{\varphi}\rangle + \langle\tilde{\phi}, (t\,(\partial_{q^j} s) + u\,(\partial_{q^j} r))\,\tilde{\pi}\rangle + \langle\tilde{\pi}, u\,(\partial_{q^j} s)\,\tilde{\pi}\rangle\Big]\,\mathrm{d}q^j \\ &- p_j\,\mathrm{d}\Big[-\frac{1}{2}\left(\langle\tilde{\varphi}, \partial_{p_j}(t\,r)\,\tilde{\varphi}\rangle + \langle\tilde{\pi}, \partial_{p_j}(u\,s)\,\tilde{\pi}\rangle + 2\langle\tilde{\varphi}, \partial_{p_j}(t\,s)\,\tilde{\pi}\rangle\right) \\ &\quad + \langle\tilde{\varphi}, t\,(\partial_{p_j} r)\,\tilde{\varphi}\rangle + \langle\tilde{\varphi}, (t\,(\partial_{p_j} s) + u\,(\partial_{p_j} r))\,\tilde{\pi}\rangle + \langle\tilde{\pi}, u\,(\partial_{p_j} s)\,\tilde{\pi}\rangle\Big]. \end{aligned} \tag{8.42}$$

The shifting of the differential is meaningful because we aim at determining the transformations of the homogeneous variables. Let us denote these transformations by $q^j \to q^j + \chi_q^j =: \tilde{q}^j$ and $p_j \to p_j + \chi_{p,j} =: \tilde{p}_j$ where the χ–transformations are of second order in the perturbations. The symplectic potential of these transformed variables is given by

$$\begin{aligned}(p_j + \chi_{p,j})\,\mathrm{d}(q^j + \chi_q^j) &= p_j\,\mathrm{d}q^j + \chi_{p,j}\,\mathrm{d}q^j + p_j\,\mathrm{d}\chi_q^j + \mathcal{O}(\chi^2) \\ &= p_j\,\mathrm{d}q^j + \chi_{p,j}\,\mathrm{d}q^j - \mathrm{d}p_j\,\chi_q^j + \mathcal{O}(\chi^2) \end{aligned} \tag{8.43}$$

where in the second line we shifted the exterior derivative from χ_q^j on p_j by omitting a total exterior differential. Consequently, it is possible to directly read off the transformations from equation (8.42). Before, we use the known relation $u\,r - s\,t = 1$ to remodel the terms in the transformations. Eventually, this gives

$$\begin{aligned}\tilde{q}^j = q^j - \frac{1}{2}\Big(&\langle\tilde{\varphi}, (t\,(\partial_{p_j} r) - r\,(\partial_{p_j} t))\tilde{\varphi}\rangle + \langle\tilde{\pi}, (u\,(\partial_{p_j} s) - s(\partial_{p_j} u))\tilde{\pi}\rangle \\ &+ \langle\tilde{\pi}, (u(\partial_{p_j} r) - r(\partial_{p_j} u) + t(\partial_{p_j} s) - s(\partial_{p_j} t))\tilde{\phi}\rangle\Big) \end{aligned} \tag{8.44}$$

$$\begin{aligned}\tilde{p}_j = p_j + \frac{1}{2}\Big(&\langle\tilde{\varphi}, (t\,(\partial_{q^j} r) - r\,(\partial_{q^j} t))\tilde{\varphi}\rangle + \langle\tilde{\pi}, (u\,(\partial_{q^j} s) - s(\partial_{q^j} u))\tilde{\pi}\rangle \\ &+ \langle\tilde{\pi}, (u(\partial_{q^j} r) - r(\partial_{q^j} u) + t(\partial_{q^j} s) - s(\partial_{q^j} t))\tilde{\varphi}\rangle\Big). \end{aligned} \tag{8.45}$$

It is easy to invert these transformations as the additional terms χ are already of second order in the perturbations. Hence, we replace all occurings of the homogeneous variabales in these terms by the dashed homogeneous variables. This yields in the truncated scheme that

$$q^j = \tilde{q}^j - \chi_q^j(\tilde{q}, \tilde{p}), \quad p_j = \tilde{p}_j - \chi_{p,j}(\tilde{q}, \tilde{p}). \tag{8.46}$$

To confine the possible transformations, we plug these results into the Hamilton function and develop the latter up to second order in the perturbations. As the perturbative Hamilton function H_{pert} is already of second order, it is allowed to simply replace the original homogeneous variables by the dashed ones. Regarding the homogeneous Hamiltonian H_{hom} the cutting of higher order terms suggests to Taylor–expand with respect to the homogeneous degrees of freedom, namely

$$H_{\mathrm{hom}}(q, p) = H_{\mathrm{hom}}(\tilde{q}, \tilde{p}) - \frac{\partial H_{\mathrm{hom}}}{\partial q^j}(\tilde{q}, \tilde{p})\,\chi_q^j(\tilde{q}, \tilde{p}) - \frac{\partial H_{\mathrm{hom}}}{\partial p_j}(\tilde{q}, \tilde{p})\,\chi_{p,j}(\tilde{q}, \tilde{p}). \tag{8.47}$$

To write this in a compact form, we emphazise that the transformations χ_q^j include derivatives of

the operators (r, s, t, u) with respect to p_j while the $\chi_{p,j}$ contain their derivatives with respect to q^j. With the respective opposite derivative of the homogeneous Hamiltonian as a prefactor, this makes the homogeneous Poisson brackets $\dot{O} = \{H_{\mathrm{hom}}, O\}_{\mathrm{hom}}$ for some observable O appear such that

$$H_{\mathrm{hom}} = \tilde{H}_{\mathrm{hom}} - \frac{1}{2}\left(\langle\tilde{\varphi}, (t\,\dot{r} - r\,\dot{t}\,)\,\tilde{\varphi}\rangle + \langle\tilde{\pi}, (u\,\dot{s} - s\,\dot{u})\,\tilde{\pi}\rangle + \langle\tilde{\pi}, (u\,\dot{r} - r\,\dot{u} + t\,\dot{s} - s\,\dot{t}\,)\,\tilde{\varphi}\rangle\right)$$

where all functions on the right hand side are evaluated at $\tilde{q}, \tilde{p}$. Accordingly from the definition of H_{pert} in equation (8.2), and with the fact that the transformations of the inhomogeneous degrees of freedom mix up configuration and momentum variables, we obtain H_{pert} in terms of the new fields $(\tilde{\varphi}, \tilde{\pi})$. In order to unify the notation, we introduce the functions and operators

$$b(a) := a^{-3}, \quad c(a) := a, \quad w(a)^2 := -a\Delta + m^2a^3. \tag{8.48}$$

In these expressions, it is allowed to replace a by $\tilde{a}$ in agreement with the truncation after the second order in the perturbations. This gives for the perturbative part of the Hamiltonian in terms of the new fields

$$H_{\mathrm{pert}} = \frac{1}{2}\left(\langle\tilde{\varphi}, (t^2b + r^2\omega^2)\,\tilde{\varphi}\rangle + \langle\tilde{\pi}, (u^2b + s^2\omega^2)\,\tilde{\pi}\rangle + 2\langle\tilde{\pi}, (ubt + s\omega^2r)\tilde{\varphi}\rangle\right)$$

where all functions depend on $\tilde{q}, \tilde{p}$. In total, the second order contributions of the transformed Hamilton function are given by

$$\begin{aligned}(H_{\mathrm{hom}} - \tilde{H}_{\mathrm{hom}}) + H_{\mathrm{pert}} = {}& \frac{1}{2}\langle\tilde{\varphi}, (t^2b + r^2w^2 - (t\dot{r} - r\dot{t}))\,\tilde{\varphi}\rangle + \frac{1}{2}\langle\tilde{\pi}, (u^2b + s^2w^2 - (u\dot{s} - s\dot{u}))\,\tilde{\pi}\rangle \\ & + \langle\tilde{\pi}, (ubt + sw^2r - \frac{1}{2}(u\dot{r} - r\dot{u} + t\dot{s} - s\dot{t}))\,\tilde{\varphi}\rangle.\end{aligned} \tag{8.49}$$

The last term is ill–defined on any Fock space, hence its exterior round bracket must vanish. The round bracket of the second contribution is supposed to be a positive operator such that the model admits a positive kinetic energy contribution. We denote it by d^2, and it is allowed to be a function of all the homogeneous variables (q, p) as well as of the Laplace–Beltrami operator Δ. The round bracket of the first contribution is accordingly required to be of the form $d^2(-\Delta + \tilde{m}^2)$ where $\tilde{m}^2$ is a function of the homogeneous variables to be determined. In fact, this will guarantee that d^2 appears as a global factor of the perturbative Hamiltonian which leaves us with a Hamiltonian density of standard form with constant coefficients for the Laplacian Δ such that the Hilbert–Schmidt condition is satisfied.

8.1.5. Concrete Choice and Application

To make these considerations more explicit, let us now consider the simplest choice for the operators (r, s, t, u) in accordance with the above requirements. These are that

(i) none of the operators (r, s, t, u) depends on Δ, and

(ii) d does not depend on Δ.

This selection is in fact unique and provides the following solutions. First, it implies that s must vanish because otherwise d^2 appearing in the kinetic term in equation (8.49) would contain a Δ

through w^2. Consequently, it holds true that $r\,u = 1$ and hence the whole round bracket of the kinetic term reduces to $d^2 = u^2 b$. Requiring that the mixed term in equation (8.49) vanishes, we obtain a direct algebraic solution for the operator t, namely

$$t = -\frac{\dot{u}}{u^2 b}. \tag{8.50}$$

Note that we freely interchange the order of the operators as they are commuting. Eventually, we consider the first line and recall that the operator in the round brackets must equal $d^2(-\Delta + \tilde{m}^2)$ where $\tilde{m}(\tilde{q}, \tilde{p})$ denotes an effective mass term which depends on the dashed variables but not on the Laplace operator. With the above choices, it is straightforward to compute that this operator is given by

$$d^2 = \frac{1}{\tilde{a}}, \quad \tilde{m}(\tilde{a}, \dot{\tilde{a}})^2 = m^2\tilde{a}^2 - \ddot{\tilde{a}}\tilde{a} - \dot{\tilde{a}}^2. \tag{8.51}$$

Thus, it is finally achievable to make the Hamilton symbol $H_{\mathrm{pert}}(\tilde{q}, \tilde{p})$ well–defined for all representations $\pi_{\tilde{a}}$ for all $\tilde{a} \in \mathbb{R}^+$. Through the dependence of $\tilde{m}^2$ on the velocity and the acceleration of the scale factor, the mass term actually depends on the momentum $\tilde{p}_a$. Hence, the coupling between the homogeneous and the perturbative sector is now provided by both the canonical variable and its conjugate momentum. Since these represent non–commuting operators in a quantum theory, the Born–Oppenheimer method is no longer available here. We are forced into the space adiabatic generalization to which we will finally come in the next section. Before we move on, let us make one important remark.

8.1.6. Discussion

One can see that the new mass square in equation (8.51) is *not* manifestly positive. With the specific choices made here, there is no freedom left to change this without making the coefficients (r, s, t, u) also depend on Δ. Whether this can be improved by exploiting the complete freedom for those operators will be left for future research.

In this respect, we draw the attention to the work by Elizaga Navascués, Mena Marugán, and Thiemann (2019). 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. Furthermore, the mass squared is a generic function of the homogeneous degrees of freedom. A prominent example for these kinds of Hamilton functions is the Mukhanov–Sasaki Hamiltonian. Hence, they are precisely in the situation arrived at above after the (almost) canonical transformations (exact up to second order). The analysis by Elizaga Navascués, Mena Marugán, and Thiemann (2019) 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 procedure has the advantage 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.

Unfortunately however, their strategy does not allow for an algebraic solution (at least in the most generic FLRW case). Rather it is necessary to solve a system consisting of two non–linear

(but semi–linear) first order partial differential equations for complex coefficient operators coming from the Hamiltonian vector field of H_{hom}. These equations 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 (Fulling 1989), the other determines an otherwise free phase. While these partial differential equations are well posed and can be solved in principle by the method of characteristics, it is generally very hard to solve the system explicity given the detailed form of H_{hom}. This however is a prerequisite to quantize the homogeneous sector as well. Thus for our purposes, we stick to the method sketched above, although the possibility to ensure the positivity of the mass squared is very attractive. We deal with the complications that arise for negative mass squared terms more explicitely in chapter 9.

There is is also another independent reason for why the approach by Elizaga Navascués, Mena Marugán, and Thiemann (2019) is 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 we simply assure the Hilbert–Schmidt condition. To see this, suppose that the symbol $K(a)$ that we derived in equation (8.26) is of Hilbert–Schmidt type and only depends on a. Then, the vector $\hat{\boldsymbol{H}}_{\text{pert}}(\hat{p}_a\Omega)$ can be computed using the explicit representation of $\hat{p}_a\Omega$ in equation (8.28). After shifting the annihilation operator due to the Hamilton operator to the right side of the resulting operator, we obtain

$$\hat{\boldsymbol{H}}_{\text{pert}}(\hat{p}_a\Omega) = -i\,\hat{\mathcal{W}}(a^{-3})\sum_{k\in\mathbb{k}}\widehat{\boldsymbol{b}^*}(a,f_k)\left(\hat{\omega}(a)\,\hat{K}(a)\,\widehat{\boldsymbol{b}^*}(a)\right)(f_k)\,\Omega \tag{8.52}$$

where $\hat{\mathcal{W}}$ represents a Weyl quantization. The operator symbol $\omega(a)K(a)$ is given using equation (8.26) by $\partial_a\omega(a)$ which grows like $|k|$ for large $|k|$ if the coefficient in front of the Laplace operator depends on the scale factor. Even if the Laplace operator does not carry an a–dependent prefactor, the resulting expression decays at most like $1/|k|$. Hence, the infinite sum over all the k's and this fall off property of the above operator prevents $(\hat{\boldsymbol{H}}_{\text{pert}}\,\hat{p}_a)$ to be a well–defined operator on Fock space. By itself this is not a problem because we want to consider the spectrum of $\hat{\boldsymbol{H}} = \hat{\mathcal{W}}(\boldsymbol{H})$ rather than $\hat{\mathcal{W}}(\boldsymbol{H}_{\text{pert}})$ which does not require to have the commutator $[\,\hat{p}_a,\hat{\boldsymbol{H}}_{\text{pert}}]$ defined on the Fock space. Nevertheless, it would be a convenient property to have. Thereby, we recall that once $\hat{\boldsymbol{H}}$ can be constructed as a self–adjoint operator, the existence of a dense and invariant domain is granted, see (Reed and Simon 1975a,b).

8.2. Cosmological Perturbations with Dust

In this section, we finally apply SAPT to a model which is very similar to the one introduced at the beginning of section 8.1. According to our discussion there, we will first determine a suitable transformation of second order in the perturbative fields in order to obtain a well–defined quantum field theory to which we can apply SAPT. Note again that the following section relies and is partially taken from (Schander and Thiemann 2019b).

8.2.1. The Hamilton Function

Following on from the previous section, we consider the four–dimensional space time manifold $\mathcal{M} \cong \mathbb{R} \times \mathbb{T}^3$ where the three–torus has side lengths 1 in all three directions although one can of course choose the lenghts completely arbitrarily. We identify points and coordinates in $\mathcal{M}$ and denote them with with lowercase letters (t, x). Our model consists of a purely homogeneous and isotropic geometry with a scale factor a as its only dynamical degree of freedom. We include the homogeneous real and timelike scalar dust field u with energy density ρ in order to deparametrize the theory. For the matter sector of the system, we choose a real scalar field $\Phi(t, x)$ of Klein–Gordon type with mass $m \in \mathbb{R}^+$ and coupling constant $\lambda \in \mathbb{R}^+$. In constrast to the model in section 8.1, we do not split the Klein–Gordon field into its purely homogeneous and inhomogeneous parts. The split in the last section served the purpose to show that the introduced transformations can be found with at least two degrees of freedom in the homogeneous sector, i.e., the scale factor *and* the homogeneous scalar field. In fact, such transformations can be found with even more homogeneous degrees of freedom. Here, we can restrict to one homogeneous variable – the scale factor – and our discussion will be hence more explicit. Since we use the dust field to deparametrize the theory, a homogeneous scalar field would not serve this purpose either.

Following the results by Halliwell and Hawking (1987) and in analogy to the results in (8.1), the action $S = S_{\text{hom}} + S_{\text{pert}}$ is given by

$$\begin{aligned} S_{\text{hom}}[a, u] &= \int_{\mathbb{R}} \mathrm{d}t \Big(-\frac{3a\,\dot{a}^2}{\kappa} - \frac{\Lambda}{\kappa} a^3 + a^3 \frac{\rho}{2} \left(\dot{u}^2 - 1 \right) \Big), \\ S_{\text{pert}}[a, \Phi] &= \frac{1}{2\lambda} \int_{\mathbb{R}\times\mathbb{T}^3} \mathrm{d}t\, \mathrm{d}x\, a^3 \Big(\dot{\Phi}^2 - \frac{1}{a^2} \Phi \left(-\Delta + a^2 m^2 \right) \Phi \Big) \end{aligned} \tag{8.53}$$

where we additionally introduced a cosmological constant $\Lambda \in \mathbb{R}^+$. Note that there is no $\sqrt{\tilde{h}^0}$ appearing anymore since the latter evaluates to one for the three–torus. $\Delta := D_a D^a$ is the Laplace–Beltrami operator on the three–torus.

We perform a Legendre transformation with the Lagrange function and density defined by $S = \int \mathrm{d}t\, L = \int \mathrm{d}t\, \mathrm{d}x\, \mathcal{L}$, and introduce the conjugate momenta

$$P_a := \frac{\partial L}{\partial \dot{a}} = -\frac{6}{\kappa} a \dot{a}, \quad \Pi_\Phi := \frac{\partial \mathcal{L}}{\partial \dot{\Phi}} = \frac{a^3}{\lambda} \dot{\Phi}. \tag{8.54}$$

Due to the dust field, the linear constraints can be solved immediately by using a reduced phase space scheme. As a consequence, the system has a physical Hamilton function $H = H_{\text{hom}} + H_{\text{pert}}$ with

$$H = -\frac{\kappa}{12} \frac{P_a^2}{a} + \frac{\Lambda}{\kappa} a^3 + \frac{\lambda}{2a^3} \int_{\mathbb{T}^3} \mathrm{d}x \Big(\Pi_\Phi^2 + \frac{a^4}{\lambda^2} \Phi \left(-\Delta + a^2 m^2 \right) \Phi \Big). \tag{8.55}$$

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

$$\{a, P_a\} = 1, \quad \{\Phi(f_1), \Pi_\Phi(f_2)\} = \int_{\mathbb{T}^3} \mathrm{d}x\, f_1(x) f_2(x) \tag{8.56}$$

where $f_1, f_2 \in C_0^\infty(\mathbb{T}^3)$ are two smearing functions. All other Poisson brackets vanish. To make

the space adiabatic scheme work at the technical level, we define the ratio of κ and λ as the dimensionless perturbative parameter $\varepsilon^2 := \frac{\kappa}{\lambda}$. As it turns out (see (Schander and Thiemann 2019a)), it is indeed reasonable to identify the homogeneous and isotropic degrees of freedom with a heavy centre of mass mode and to consequently define $p_a := \varepsilon P_a$ as a rescaled momentum. To simplify notation, we also define a rescaled cosmological constant which we assume still to be very small, namely $\tilde{\Lambda} := \frac{\Lambda}{\varepsilon^2}$. We divide the Hamiltonian by the constant λ, keep this in mind but continue to denote the Hamiltonian by the same symbol. Its homogeneous part is given by

$$H_{\text{hom}} = -\frac{1}{12}\frac{p_a^2}{a} + \tilde{\Lambda} a^3, \tag{8.57}$$

and similar to the oscillator example, we have $\{a, p_a\} = \varepsilon$. As anticipated in the previous section, the scheme requires to perform additional transformations of the fields in order have a well–defined quantum field theory.

8.2.2. Almost Canonical Transformation

The inhomogeneous part of the Hamilton function in equation (8.55) depends on the effective frequency operator $\omega(a) = \sqrt{-a^4\Delta + m^2 a^6}$. Recall from the previous section that the a–dependence of the Laplace term in $\omega(a)$ prevents the quantum field theory of (Φ, Π_Φ) from having unitarily equivalent representations for different values of the scale factor. In the same lines, this section derives a transformation which is canonical up to second order in the perturbative fields. Therefore, consider the symplectic one–form Θ on the tangent space of the total phase space. In coordinate representation, in which $\mathrm{d}a$ and $\mathrm{d}\Phi$ represent the standard one–forms for the homogeneous and the inhomogeneous phase spaces respectively, we have that Θ is given by

$$\Theta = P_a\,\mathrm{d}a + \int_{\mathcal{B}} \mathrm{d}x\,\Pi_\Phi(x)\,\mathrm{d}\Phi(x) = \frac{1}{\varepsilon}\,p_a\,\mathrm{d}a + \int_{\mathbb{T}^3} \mathrm{d}x\,\Pi_\Phi(x)\,\mathrm{d}\Phi(x). \tag{8.58}$$

As an ansatz for the transformations of the inhomogeneities, inspired by the results in section 8.1, we employ

$$\tilde{\Phi} := a\cdot\Phi,\;\; \tilde{\Pi}_\Phi := \frac{\Pi_\Phi}{a} + a\,g(a,p_a)\,\Phi \quad\Rightarrow\quad \Phi = \frac{\tilde{\Phi}}{a},\;\; \Pi_\Phi = a\,(\tilde{\Pi}_\Phi - g(a,p_a)\,\tilde{\Phi}) \tag{8.59}$$

where $g(a, p_a)$ is a real–valued function that needs to be determined by our condition on the field theory. Besides, the following abbreviations will prove to be useful:

$$A := \int_{\mathbb{T}^3} \mathrm{d}x\,\Phi(x)^2 = \frac{1}{a^2}\int_{\mathbb{T}^3} \mathrm{d}x\,\tilde{\Phi}(x)^2 =: \frac{\tilde{A}}{a^2}, \tag{8.60}$$

$$B := \int_{\mathbb{T}^3} \mathrm{d}x\,\Pi_\Phi(x)\Phi(x) = \int_{\mathbb{T}^3} \mathrm{d}x\,\tilde{\Pi}_\Phi(x)\tilde{\Phi}(x) - g(a,p_a)\tilde{A} =: \tilde{B} - g\,\tilde{A}. \tag{8.61}$$

We insert the transformations (8.59) into the symplectic potential Θ and use the definitions (8.60) and (8.61). The product rule for the differential one–form which we apply on $\frac{\tilde{\Phi}}{a}$ and omitting total

differentials then yields

$$\Theta = \left(\frac{1}{\varepsilon}\, p_a - \frac{1}{a}\tilde{B} + \frac{g}{a}\tilde{A}\right) \mathrm{d}a + \int_{\mathbb{T}^3} \mathrm{d}x\, \tilde{\Pi}_\Phi\, \mathrm{d}\tilde{\Phi} + \frac{\tilde{A}}{2}\mathrm{d}g. \tag{8.62}$$

Since g depends solely on a and p_a, we can write $\mathrm{d}g = g_{,a}\,\mathrm{d}a + g_{,p_a}\,\mathrm{d}p_a$, where the comma corresponds to the derivative with respect to the given variable. The term proportional to $\mathrm{d}a$ fits nicely into the first bracket in equation (8.62). For the second term, we use that total differentials vanish, and by cutting the theory after the second order in the scalar field variables, the symplectic potential has the form

$$\Theta = \left(\frac{1}{\varepsilon}\, p_a - \frac{1}{a}\tilde{B} + \frac{g}{a}\tilde{A} + \frac{1}{2}g_{,a}\,\tilde{A}\right) \mathrm{d}\left(a - \frac{1}{2}\varepsilon g_{,p_a}\,\tilde{A}\right) + \int_{\mathbb{T}^3} \mathrm{d}x\, \tilde{\Pi}_\Phi\, \mathrm{d}\tilde{\Phi}. \tag{8.63}$$

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

$$\tilde{p}_a := p_a + \varepsilon\left(-\frac{1}{a}\tilde{B} + \frac{g}{a}\tilde{A} + \frac{1}{2}g_{,a}\,\tilde{A}\right), \quad \tilde{a} := a - \frac{1}{2}\varepsilon g_{,p_a}\,\tilde{A}. \tag{8.64}$$

With these dashed variables, the symplectic potential regains its original form. It remains to determine the function $g(a, p_a)$ and to verify whether the Hamilton function transforms into a well–defined function with respect to the new variables. In order to express the Hamilton function in terms of them, we need to invert the rules (8.64). It proves to be beneficial to directly employ an explicit representation for the function g. An educated guess is

$$g(a, p_a) = -\frac{\varepsilon}{6}\frac{p_a}{a}. \tag{8.65}$$

Its derivatives with respect to p_a serve for determining a as a function of the dashed variables with equation (8.64). Multiplying the latter by a, using an algebraic solution formula for quadratic equations and cutting again after second order in the perturbative fields gives the second relation in equation (8.66) as a solution for a. To determine p_a as a function of $\tilde{a}$ and $\tilde{p}_a$, we insert the solution for $a(\tilde{a}, \tilde{p}_a)$ into the first relation in (8.64) and Taylor expand the function up to second order in the perturbation fields. This yields

$$p_a = \tilde{p}_a + \varepsilon\frac{1}{\tilde{a}}\tilde{B} + \frac{\varepsilon^2}{12}\frac{\tilde{p}_a}{\tilde{a}}\tilde{A}, \quad a = \tilde{a} - \frac{\varepsilon^2}{12\tilde{a}}\tilde{A}. \tag{8.66}$$

In a first step, we compute the homogeneous part of the Hamilton function (8.57) in terms of the dashed variables and eventually compare it with the perturbative part. We use the rules (8.66) and Taylor expand again up to second order in the perturbation fields. For the homogeneous part, now including also second order contributions, we get the following result:

$$\tilde{H}_{\mathrm{hom}} = -\frac{1}{12}\frac{\tilde{p}_a^2}{\tilde{a}} + \tilde{\Lambda}\tilde{a}^3 - \frac{\varepsilon}{6}\frac{\tilde{p}_a}{\tilde{a}^2}\tilde{B} - \frac{\varepsilon^2}{48}\frac{\tilde{p}_a^2}{\tilde{a}^3}\tilde{A} - \frac{\Lambda}{4}\tilde{a}\tilde{A}. \tag{8.67}$$

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

is given in terms of the dashed variables by omitting any contributions of third order and higher in the fields

$$\tilde{H}_{\mathrm{pert}} = \frac{1}{2\tilde{a}} \int_{\mathbb{T}^3} \mathrm{d}x \left(\tilde{\Pi}_{\Phi}^2 + \tilde{\Phi} \left(-\Delta + \tilde{a}^2 m^2 \right) \tilde{\Phi} \right) + \frac{\varepsilon}{6} \frac{\tilde{p}_a}{\tilde{a}^2} \tilde{B} + \frac{\varepsilon^2}{72} \frac{\tilde{p}_a^2}{\tilde{a}^3} \tilde{A}. \tag{8.68}$$

We observe that the a–dependence of the Laplace term has indeed vanished and a global factor $\tilde{a}^{-1}$ has appeared for the classical Klein–Gordon Hamilton function. Besides, the transformation yields new terms which indeed cancel the anomalous contribution proportional to $\tilde{B}$ in the dashed homogeneous Hamilton function (8.67). In total, the Hamiltonian $\tilde{H} = \tilde{H}_{\mathrm{hom}} + \tilde{H}_{\mathrm{pert}}$ gives rise to two supplementary, independent contributions that depend on $\tilde{A}$. Recalling that $\tilde{A} = \int \mathrm{d}x\, \Phi^2$, they yield additional contributions to an effective mass function $\tilde{M}(\tilde{a}, \tilde{p}_a)$, namely

$$\tilde{H} = -\frac{1}{12} \frac{\tilde{p}_a^2}{\tilde{a}} + \tilde{\Lambda} \tilde{a}^3 + \frac{1}{2\tilde{a}} \int_{\mathbb{T}^3} \mathrm{d}x \left(\tilde{\Pi}_{\Phi}^2 + \tilde{\Phi} \left(-\Delta + \tilde{M}(\tilde{a}, \tilde{p}_a)^2 \right) \tilde{\Phi} \right), \tag{8.69}$$

$$\text{with } \tilde{M}(\tilde{a}, \tilde{p}_a)^2 = \left(m^2 - \frac{\Lambda}{2} \right) \tilde{a}^2 - \frac{\varepsilon^2}{72} \frac{\tilde{p}_a^2}{\tilde{a}^2}. \tag{8.70}$$

The Laplace term in the perturbative part of this Hamilton function no longer depends on the scale factor. After a quantization of the fields, the Fock representations are consequently unitarily equivalent for different background configurations. This allows to finally apply the space adiabatic perturbation scheme. However, the effective mass square function in equation (8.70) is indefinite, thus leading to tachyonic instabilities for certain regions in the slow phase space Γ_{hom}. We refer to section 9.2 where we present several strategies for how to deal with this issue. Here, we perform an additional canonical transformation with respect to the homogeneous variables only such that the effective mass squared becomes positive definite. Therefore, we define a set of constant parameters

$$\mu^2 := m^2 - \frac{\Lambda}{2}, \quad \tau^2 := \frac{\varepsilon^2}{72}, \quad \sigma^2 := \frac{\tau^2}{\mu^2}. \tag{8.71}$$

We assume the constant μ^2 to be positive such that σ is in the reals. The effective mass value then becomes $\tilde{M}^2 =: \mu^2 \tilde{a}^2 - \tau^2 \frac{\tilde{p}_a^2}{\tilde{a}^2}$. We also choose a new canonical pair (b, p_b) according to

$$\tilde{a} =: \sqrt{b^2 + \sigma^2 \frac{p_b^2}{b^2}} =: \beta(b, p_b), \quad \tilde{p}_a =: \tilde{a}\, \frac{p_b}{b}. \tag{8.72}$$

Accordingly, the effective mass square function is simply given by $\tilde{M}^2 = \mu^2 b^2$ which is positive for any $b \in \mathbb{R}$. By this choice, we implicitely limit the original phase space in terms of $(\tilde{a}, \tilde{p}_a)$ to a restricted domain. The starting point for SAPT is the Hamilton function in terms of the new variables given by

$$H = -\frac{1}{12} \beta \frac{p_b^2}{b^2} + l^3 \tilde{\Lambda} \beta^3 + \frac{1}{2\beta} \int_{\mathbb{T}^3} \mathrm{d}x \left(\tilde{\Pi}_{\Phi}^2 + \tilde{\Phi} \left(-\Delta + \mu^2 b^2 \right) \tilde{\Phi} \right). \tag{8.73}$$

To quantize the theory, we employ the standard Schrödinger representation for the geometric variables (b, p_b) labeling quantum operators by hats, i.e., $\hat{b}$ and $\hat{p}_b$ for the canonical quantum operators. We recall that b and p_b arose from the rescaled variables $\tilde{a}$ and $\tilde{p}_a$ such that the canonical

commutation relation is given by $[\hat{b}, \hat{p}_b] = i\varepsilon \hat{1}_{\text{hom}}$. Regarding the ordering of non–commuting operators, we employ the symmetric Weyl quantization procedure for the homogeneous sector. The Hilbert space is simply $L^2(\mathbb{R}, \mathrm{d}b)$ with the standard measure on $\mathbb{R}$.

For the fast Klein–Gordon field $\tilde{\Phi}$, we choose a standard Fock representation on the compact manifold $\mathbb{T}^3$. Therefore, consider the one–particle Hilbert space $\mathcal{H}_{\mathbb{T}^3} = L^2(\mathbb{T}^3, \mathrm{d}x)$ on $\mathbb{T}^3$. The almost canonical transformations from above guarantee that all Fock representations $\pi_{(b,p_b)}$ for different (b, p_b) are mutually unitarily equivalent at least up to second order in the field perturbations. We mark operators acting on $\mathcal{F}_{\text{s}}(\mathcal{H}_{\mathbb{T}})$ with bold letters such that the basic field operators are $\boldsymbol{\Phi}(f_1)$ and $\boldsymbol{\Pi}_{\Phi}(f_2)$ for some smooth test functions $f_1, f_2 \in C_0^{\infty}(\mathbb{T}^3)$. The Fock space $\mathcal{F}_{\text{s}}$ consists of sequences $\{\psi_{(n)}\}_{n\geq 0}$ of totally symmetric functions with n variables. The canonical commutation relations are given by

$$[\boldsymbol{\Phi}(f_1), \boldsymbol{\Pi}_{\Phi}(f_2)]_{\text{pert}} = i\,\langle f_1, f_2\rangle\, \mathbf{1}_{\text{pert}}. \tag{8.74}$$

In order to define the quantum theory of the whole system, we introduce the total Hilbert space as the topological tensor product $\mathcal{H} := \mathcal{H}_{\text{hom}} \otimes \mathcal{H}_{\text{pert}} = L^2(\mathbb{R}, \mathrm{d}b) \otimes \mathcal{F}_{\text{s}}$. With these prerequisites, the Hamilton operator $\hat{\boldsymbol{H}}$ acting on a dense subset $\mathcal{D} \subset \mathcal{H}$ of the total Hilbert space has the form

$$\begin{aligned}\hat{\boldsymbol{H}} = \hat{\mathcal{W}}\left(-\frac{1}{12}\beta\,\frac{p_b^2}{b^2} + \tilde{\Lambda}\beta^3\right) \otimes \mathbf{1}_{\text{pert}} + \frac{1}{2}\hat{\mathcal{W}}(\beta^{-1}) \otimes \int_{\mathbb{T}^3} \mathrm{d}x\, \boldsymbol{\Pi}_{\Phi}(x)^2 \\ + \frac{1}{2}\hat{\mathcal{W}}(\beta^{-1}) \otimes \int_{\mathbb{T}^3} \mathrm{d}x\, \boldsymbol{\Phi}(x)(-\Delta\boldsymbol{\Phi})(x) + \frac{\mu^2}{2}\hat{\mathcal{W}}(\beta^{-1}b^2) \otimes \int_{\mathbb{T}^3} \mathrm{d}x\, \boldsymbol{\Phi}(x)^2.\end{aligned} \tag{8.75}$$

8.2.3. Checking of the Conditions

We check the conditions (C1) – (C4) before we apply SAPT. Regarding (C1), it is clear that the Hilbert space has the form of a tensor product $\mathcal{H} = \mathcal{H}_{\text{hom}} \otimes \mathcal{H}_{\text{pert}}$ with $\mathcal{H}_{\text{hom}} = L^2(\mathbb{R}, \mathrm{d}b)$ and $\mathcal{H}_{\text{pert}} = \mathcal{F}_{\text{s}}$ and the latter factor is also a separable Hilbert space. For condition (C2), let us consider the formal quantization of the Hamilton function in equation (8.73) with respect to the inhomogeneous field perturbations only, or in other terms, the Wigner–Weyl transform of the Hamilton operator (8.75) with respect to the slow subsector. This gives rise to the operator–valued function on the slow phase space

$$\boldsymbol{H}(b, p_b) := \left(-\frac{1}{12}\beta\frac{p_b^2}{b^2} + \tilde{\Lambda}\beta^3\right)\mathbf{1}_{\text{pert}} + \frac{1}{2\beta}\int_{\mathbb{T}^3} \mathrm{d}x\Big(\tilde{\boldsymbol{\Pi}}_{\Phi}^2 + \tilde{\boldsymbol{\Phi}}\,(-\Delta + \mu^2 b^2)\,\tilde{\boldsymbol{\Phi}}\Big). \tag{8.76}$$

We represent the Hamiltonian in terms of annihilation and creation operators $\boldsymbol{a}(b, f)$ and $\boldsymbol{a}^*(b, f)$ for some one particle state $f \in L^2(\mathbb{T}^3, \mathrm{d}x)$ and for some fixed $b \in \mathbb{R}$. Therefore, we use the b–dependent representation map $\pi_b : \mathcal{A}_Q \to \mathcal{L}(\mathcal{F}_{\text{s}})$ between the field Weyl algebra $\mathcal{A}_Q$ and the space of linear operators on Fock space $\mathcal{F}_{\text{s}}$. With the one–particle frequency operator $\omega(b) := \sqrt{-\Delta + \mu^2 b^2}$, the annihilation operator is given by

$$\boldsymbol{a}(b, f) := \frac{1}{\sqrt{2}}\,\pi_b\left[\big(\sqrt{\omega(b)}\tilde{\boldsymbol{\Phi}}\big)(f) - i\big(\sqrt{\omega(b)}^{-1}\tilde{\boldsymbol{\Pi}}_{\Phi}\big)(f)\right]. \tag{8.77}$$

The canonical commutation relations become $[\boldsymbol{a}(b, f_1), \boldsymbol{a}^*(b, f_2)] = \mathbf{1}_{\text{pert}} \cdot \int \mathrm{d}x\, f_1(x)\, f_2(x)$. We consider the plane waves $f_k = \exp(ik \cdot x)$ with $k \in \Sigma := 2\pi\mathbb{Z}^3$ as an orthonormal basis of

the Hilbert space $\mathcal{H}_{\mathbb{T}^3}$. We denote the annihilation and creation operators with respect to the basis states by $\boldsymbol{a}_k(b)$ and $\boldsymbol{a}_k^*(b)$ such that $[\boldsymbol{a}_k(b), \boldsymbol{a}_{k'}^*(b)] = \delta_{k,k'}\mathbf{1}_{\text{pert}}$. The Laplace–Beltrami operator has corresponding eigenvalues $-\Delta f_k =: k^2 f_k$ such that the frequency operator evaluates to $\omega(b, k^2) := (k^2 + \mu^2 b^2)^{1/2}$ when applied to f_k. The Hamilton symbol (8.76) with normal ordering is accordingly given by

$$\boldsymbol{H}(b, p_b) = \left(-\frac{1}{12}\beta\frac{p_b^2}{b^2} + \tilde{\Lambda}\beta^3\right)\mathbf{1}_{\text{pert}} + \frac{1}{\beta}\sum_{k\in\Sigma}\omega(b, k^2)\,\boldsymbol{a}_k^*(b)\,\boldsymbol{a}_k(b). \tag{8.78}$$

Condition (C2) requires $\boldsymbol{H}(b, p_b)$ to be a symbol function in one of the classes S_ρ^m for which $\boldsymbol{H}(b, p_b)$ must be a bounded operator on $\mathcal{F}_{\text{s}}$. Like for the finite dimensional cases, this is a priori not satisfied since the number operator can have infinite values for infinitely excited states. Besides, $\boldsymbol{H}(b, p_b)$ is not a bounded function with respect to b and p_b. The situation is very similar to the one encountered in the examples in chapters 6 and 7. To fix this problem, one may proceed in the same way as in section 6.8 and introduce an auxiliary Hamilton symbol $\boldsymbol{H}_{\text{aux}}$ by truncating the sum over k in equation (8.78) and by restricting this symbol further to a certain cut–off energy. The resulting symbol lies in the symbol class S_0^0 and satisfies hence condition (C2). This is again at the cost of creating a new, physically inequivalent problem. Otherwise, one can stick to the original Hamilton symbol at the cost of relinquishing convergence of the resulting adiabatic perturbation series. In the following, we will adopt the second path, and point out again that for the first approach, one would need to investigate the convergence of the adiabatic series by independent means.

To check the gap condition (C3), let us evaluate the eigenstates associated with the symbol $\boldsymbol{H}(b, \rho_b)$. Since the mode vectors k are discrete, the eigenvalues of $\boldsymbol{H}$ are discrete as well. For each pair of annihilation and creation operators $\boldsymbol{a}_k(b)$ and $\boldsymbol{a}^*(b)$, there is a natural vacuum state $\Omega(b)$ defined by the requirement $\boldsymbol{a}_k(b)\Omega(b) = 0$ for every $k \in \Sigma$. Any excited eigenstate $\xi_{(n)}(b)$ where (n) is a short form for the collection of its excitation numbers $\{n_k\}_{k\in\Sigma}$ results from the (n)–times application of the creation operators

$$\xi_{(n)}(b) = \prod_{k\in\Sigma}\frac{\left(\boldsymbol{a}_k^*(b)\right)^{n_k}}{\sqrt{n_k!}}\Omega(b). \tag{8.79}$$

The energy bands $E_{(n)}(b, p_b)$ are the (b, p_b)–dependent energy eigenvalues of the symbol function $\boldsymbol{H}(b, p_b)$. As the Hamiltonian depends only on the wave number k via its square k^2, it is clear that there are degenerate eigenstates. In particular, for each vector $k \in \Sigma$ there are (at least) $2^3 - 1$ vectors in Σ with the same eigenenergy. We therefore label, whenever needed, the degenerate eigenstates associated with those wave vectors by an additional degeneracy label $a = 1, \ldots, d_{(n)}$ with degeneracy number $d_{(n)} \in \mathbb{N}$. The generalized eigenvalue equation for the Klein–Gordon field problem is then given with respect to a degenerate set of eigenstates $\xi_{(n)_a}(b)$ by

$$\boldsymbol{H}(b, p_b)\xi_{(n)_a}(b) = E_{(n)}(b, p_b)\,\xi_{(n)_a}(b) \tag{8.80}$$

$$\text{with}\quad E_{(n)}(b, p_b) = -\frac{1}{12}\,\beta\,\frac{p_b^2}{b^2} + \tilde{\Lambda}\beta^3 + \frac{1}{\beta}\sum_{k\in\Sigma} n_{k,a}\,\omega(b, k^2). \tag{8.81}$$

The spectrum $\sigma(b, p_b)$ of $\boldsymbol{H}(b, p_b)$ thus consists of the set of all energy bands $\{E_{(n)}(b, p_b)\}_{(n)}$ for all possible combinations of excitation numbers (n). SAPT demands to choose an isolated subset $\sigma_\nu(b, p_b) \subset \sigma(b, p_b)$ which is uniformly separated from the remainder of the spectrum.

It appears that the energy functions depends on i) k^2 and ii) their excitation numbers n_k for any of the excited one–particle states that contributes to the total Fock state. Obviously, these energy functions $E_{(n)}(b, p_b)$ are subject to eigenvalue crossings for varying b (note that the (b, p_b)–dependent homogeneous contribution to the Hamilton symbol is the same for all energy bands and plays hence no role for the energy gap). Such overlaps are prohibited for the application of SAPT as we have presented it here, and the failure of the gap condition leads to a considerably more difficult realization of the space adiabatic scheme, see for example (Teufel 2003, Chapter 6).

One possible resort is to restrict the configuration variable b to an appropriate domain $I \subset \Gamma_{\text{hom}}$ of the homogeneous phase space after having chosen (ν), and such that the corresponding energy function $E_{(\nu)}(b, p_b)$ does not cross with any of the remaining energy bands in that region of phase space. One must then consider the such restricted phase space when it comes to quantization and hence, also for the realization of the SAPT scheme. More precisely, one considers the cotangent bundle T^*I as a phase space and uses a corresponding well–defined quantization scheme. Within the scope of this thesis, we will bypass this issue for now and focus on the formal problem of applying SAPT to the Hamilton symbol on its original domain. The corresponding quantization problem is a formidable topic for future work.

8.2.4. Space Adiabatic Construction Scheme

We construct the Moyal projector $\boldsymbol{\pi}$ and the Moyal unitary $\boldsymbol{u}$ for the inhomogeneous cosmological model with dust up to first order in perturbation theory and according to the construction steps (S1) and (S2). Accordingly, we compute the effective Hamiltonian $\boldsymbol{h}_{\text{eff,R}}$ up to second order according to the rule (S3).

(S1): Construction of the Projector Symbol $\boldsymbol{\pi}_{(1)}$

The inductive scheme suggests to construct $\boldsymbol{\pi}_{(1)} = \boldsymbol{\pi}_0 + \varepsilon\boldsymbol{\pi}_1$ choosing as initial data the symbol function

$$\boldsymbol{\pi}_0 := \sum_{a=1}^{d_{(\nu)}} \xi_{(\nu)_a}(b)\, \langle \xi_{(\nu)_a}(b), \cdot \rangle_{\mathcal{F}_{\text{s}}} \tag{8.82}$$

where $(\nu)_a = \{\nu_{k,a}\}_{k\in\Sigma}$ is the set of excitation numbers of the chosen Fock state and $a = 1, \ldots, d_{(\nu)}$ is the associated degeneracy label. The zeroth order of the conditions (S1) is satisfied trivially by construction, i.e.,

$$\boldsymbol{\pi}_0 \cdot \boldsymbol{\pi}_0 = \boldsymbol{\pi}_0, \quad \boldsymbol{\pi}_0^* = \boldsymbol{\pi}_0, \quad \boldsymbol{H} \cdot \boldsymbol{\pi}_0 - \boldsymbol{\pi}_0 \cdot \boldsymbol{H} = 0. \tag{8.83}$$

Note that the full Hamilton symbol $\boldsymbol{H}$ can be identified with a zeroth order contribution in the ε–scheme. Although β carries contributions that depend on ε, for simplicity we keep these terms as they can simply be neglected at the end. Note that the symbol $\boldsymbol{\pi}_0$ solely depends on the triad–like configuration variable b. As shown in section 6.7, the diagonal contribution to $\boldsymbol{\pi}_1$ vanishes in this case. While we can use the same formal expression for the off–diagonal part of $\boldsymbol{\pi}_1$ as for the

finite–dimensional models, namely equation (6.131), its concrete evaluation needs more care. It is necessary to evaluate the derivatives of the eigenfunctions $\xi_{(n)}(b)$ with respect to b for which we use the explicit b–dependence of the creation operators $\boldsymbol{a}_k^*(b)$ in line with equation (8.77) and relation (8.79) for the excited Fock states. Therefore, let us first define the function

$$\alpha(b,k^2) := -\frac{1}{4}\frac{\partial_b\,\omega(b,k^2)}{\omega(b,k^2)}. \tag{8.84}$$

Then, the identity $\partial_b\,\boldsymbol{a}_k(b) = -2\alpha(b,k^2)\,\boldsymbol{a}_k^*(b)$ follows from (8.77) and together with the equations $\boldsymbol{a}_k(b)\,\Omega(b) = 0$ for all $k \in \Sigma$ it implies that the derivative of the vacuum state $\Omega(b)$ is given by

$$\frac{\partial\Omega(b)}{\partial b} = \sum_{k\in\Sigma}\alpha(b,k^2)\,\boldsymbol{a}_k^*(b)\,\boldsymbol{a}_k^*(b)\,\Omega(b). \tag{8.85}$$

Given the derivatives of the creation operators and the vacuum state, it is straightforward to deduce the derivatives of the excited states $\xi_{(n)}(b)$ from equation (8.79). Therefore, we denote the state whose quantum number n_k for the wave vector k is shifted by ± 2 compared to the state $\xi_{(n)}(b)$ by $\xi_{\{..,n_k\pm 2,..\}}$. Then, the derivative of $\xi_{(n)}(b)$ is given by

$$\begin{aligned}\frac{\partial\xi_{(n)}(b)}{\partial b} &= -\sum_{k\in\Sigma}\alpha(b,k^2)\sqrt{(n_k-1)n_k}\,\frac{(\boldsymbol{a}_k^*)^{n_k-2}}{\sqrt{(n_k-2)!}}\prod_{m\in\Sigma\setminus\{k\}}\frac{(\boldsymbol{a}_m^*)^{\nu_m}}{\sqrt{n_m!}}\,\Omega(b)\\ &\quad+\sum_{k\in\Sigma}\alpha(b,k^2)\sqrt{(n_k+1)(n_k+2)}\,\frac{(\boldsymbol{a}_k^*)^{n_k+2}}{\sqrt{(n_k+2)!}}\prod_{m\in\Sigma\setminus\{k\}}\frac{(\boldsymbol{a}_m^*)^{n_m}}{\sqrt{n_m!}}\,\Omega(b)\\ &= \sum_{k\in\Sigma}\alpha(b,k^2)\left(-\sqrt{(n_k-1)n_k}\,\xi_{\{..,n_k-2,..\}}+\sqrt{(n_k+1)(n_k+2)}\,\xi_{\{..,n_k+2,..\}}\right).\end{aligned} \tag{8.86}$$

Again, we define a gauge potential $\boldsymbol{\mathcal{A}} \in C^\infty(\Lambda(\Gamma_{\mathrm{hom}})\otimes\mathcal{L}(\mathcal{H}_{\mathrm{pert}}))$ as a one–form on the homogeneous phase space Γ_{s} and with values in the linear operators on the symmetric Fock space $\mathcal{H}_{\mathrm{pert}} = \mathcal{F}_{\mathrm{s}}$. With the choice of the basis states $\{\xi_{(n)}\}$, we write for the coefficients of $\boldsymbol{\mathcal{A}}$

$$\mathcal{A}_{b(n)}^{\ (m)} = \sum_{k\in\Sigma}\alpha(b,k^2)\left(-\sqrt{n_k(n_k-1)}\,\delta_{(n)}^{\{..,m_k+2,..\}}+\sqrt{(n_k+2)(n_k+1)}\,\delta_{(n)}^{\{..,m_k-2,..\}}\right).$$

Using these coefficients, the expression for the state derivatives has a simpler form, namely

$$\frac{\partial\xi_{(n)}(b)}{\partial b} = \sum_{k\in\Sigma}\left(\mathcal{A}_{b(n)}^{\ \{..,n_k-2,..\}}\xi_{\{..,n_k-2,..\}}+\mathcal{A}_{b(n)}^{\ \{..,n_k+2,..\}}\xi_{\{..,n_k+2,..\}}\right). \tag{8.87}$$

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

$$\begin{aligned}\frac{\partial\boldsymbol{\pi}_0(b)}{\partial b} = \sum_{a=1}^{d_\nu}\sum_{k\in\Sigma}\Big(&\mathcal{A}_{b(\nu)_a}^{\ \{..,\nu_{k,a}-2,..\}}\left(\xi_{(\nu)_a}\langle\xi_{\{..,\nu_{k,a}-2,..\}},\cdot\,\rangle_{\mathcal{F}_{\mathrm{s}}}+\xi_{\{..,\nu_{k,a}-2,..\}}\langle\xi_{(\nu)_a},\cdot\,\rangle_{\mathcal{F}_{\mathrm{s}}}\right)\\ &+\mathcal{A}_{b(\nu)_a}^{\ \{..,\nu_{k,a}+2,..\}}\left(\xi_{(\nu)_a}\langle\xi_{\{..,\nu_{k,a}+2,..\}},\cdot\,\rangle_{\mathcal{F}_{\mathrm{s}}}+\xi_{\{..,\nu_{k,a}+2,..\}}\langle\xi_{(\nu)_a},\cdot\,\rangle_{\mathcal{F}_{\mathrm{s}}}\right)\Big).\end{aligned} \tag{8.88}$$

To evaluate $\boldsymbol{\pi}_1$, the Poisson bracket in equation (6.131) requires to determine the p_b–derivative of the symbol function $(\boldsymbol{H}+E_{(\nu)}\,\mathbf{1}_{\mathrm{pert}})$. This function depends on p_b via its homogeneous gravita-

tional part of $\boldsymbol{H}(b, p_b)$ and of $E_{(\nu)}$, which we define by

$$E_{\text{hom}}(b, p_b) = -\frac{1}{12}\beta(b, p_b)\frac{p_b^2}{b^2} + \tilde{\Lambda}\beta(b, p_b)^3. \tag{8.89}$$

Besides, the perturbative field contribution of the Hamilton symbol and the energy function $E_{(\nu)}$ depend on p_b via the global prefactor $\beta(b, p_b)^{-1}$, cf. equation (8.78) such that diagonal contributions from this part enter as well in the evaluation of the Poisson bracket. We denote the perturbative part of $E_{(\nu)}$ as $E_{\text{pert},(\nu)}$. In the formula for $\boldsymbol{\pi}_1$, the symbol operators $\boldsymbol{\pi}_0$ and $\partial_b \boldsymbol{\pi}_0$ select the relevant contributions in $\partial_{p_b}(\boldsymbol{H}_0 + E_{(\nu)}\mathbf{1}_{\text{pert}})$ for every $k \in \Sigma$. These restrict also the relevant contributions from $(\boldsymbol{H}^\perp - E_{(\nu)}\mathbf{1}_{\text{pert}})^{-1}$ for every k, namely to $(E_{\{..,\nu_{k,a}-2,..\}} - E_{(\nu)_a})\,\xi_{\{..,\nu_{k,a}-2,..\}}\langle\xi_{\{..,\nu_{k,a}-2,..\}}, \cdot\rangle_{\mathcal{F}_s}$ and $(E_{\{..,\nu_{k,a}+2,..\}} - E_{(\nu)_a})\,\xi_{\{..,\nu_{k,a}+2,..\}}\langle\xi_{\{..,\nu_{k,a}+2,..\}}, \cdot\rangle_{\mathcal{F}_s}$. The two energy differences appearing there, i.e., the two scalar factors, evaluate to $\mp\Delta_k := \mp\frac{2}{\Sigma}\omega(b, k^2)$. In total, this gives

$$\begin{aligned}\boldsymbol{\pi}_1 = \frac{i}{2}\sum_{a=1}^{d_{(\nu)}}\sum_{k\in\Sigma}\Big(&\mathcal{A}_{b(\nu)_a}^{\{..,\nu_{k,a}-2,..\}} C_{1,(\nu),k}\left(\xi_{(\nu)_a}\langle\xi_{\{..,\nu_{k,a}-2,..\}}, \cdot\rangle_{\mathcal{F}_s} - \xi_{\{..,\nu_{k,a}-2,..\}}\langle\xi_{(\nu)_a}, \cdot\rangle_{\mathcal{F}_s}\right)\\ &+ \mathcal{A}_{b(\nu)_a}^{\{..,\nu_{k,a}+2,..\}} C_{2,(\nu),k}\left(\xi_{(\nu)_a}\langle\xi_{\{..,\nu_{k,a}+2,..\}}, \cdot\rangle_{\mathcal{F}_s} - \xi_{\{..,\nu_{k,a}+2,..\}}\langle\xi_{(\nu)_a}, \cdot\rangle_{\mathcal{F}_s}\right)\Big)\end{aligned} \tag{8.90}$$

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

$$C_{1,(\nu),k}(b, p_b) =: \frac{1}{\Delta_k}\left(\frac{\partial E_{\text{hom}}}{\partial p_b} - \frac{1}{\beta}\frac{\partial\beta}{\partial p_b}E_{\text{pert},(\nu)}\right) + \frac{1}{\beta}\frac{\partial\beta}{\partial p_b}, \tag{8.91}$$

$$C_{2,(\nu),k}(b, p_b) := -\frac{1}{\Delta_k}\left(\frac{\partial E_{\text{hom}}}{\partial p_b} - \frac{1}{\beta}\frac{\partial\beta}{\partial p_b}E_{\text{pert},(\nu)}\right) + \frac{1}{\beta}\frac{\partial\beta}{\partial p_b}. \tag{8.92}$$

The same results can be obtained following the scheme in section 6.7. The inclusion of degenerate eigenstates and the infinite number of degrees of freedom yields

$$\boldsymbol{\pi}_1 = \frac{i}{2}\sum_{a=1}^{d_{(\nu)}}\sum_{(m)}\frac{A_{(\nu)_a(m)}}{E_{(\nu)} - E_{(m)}}\left(\xi_{(\nu)_a}\langle\xi_{(m)}, \cdot\rangle_{\mathcal{F}_s} - \xi_{(m)}\langle\xi_{(\nu)_a}, \cdot\rangle_{\mathcal{F}_s}\right) \tag{8.93}$$

where A was defined in equation (6.134). While the sum over (m) includes in principle all possible combinations of excitation numbers, the function $A_{(\nu)_a(m)}$ is only non–vanishing for a restricted number of combinations of (m). In particular, the only non–vanishing contributions are

$$\begin{aligned}\frac{A_{(\nu)_a\{...,\nu_{k,a}\pm2,...\}}}{E_{(\nu)_a} - E_{\{...\nu_{k,a}\pm2,...\}}} &= \frac{\mathcal{A}_{b(\nu)_a}^{\{...,\nu_{k,a}\pm2,...\}}}{E_{(\nu)_a} - E_{\{...,\nu_{k,a}\pm2,...\}}}\frac{\partial(E_{(\nu)_a} + E_{\{...,\nu_{k,a}\pm2,...\}})}{\partial p_b}\\ &= \pm\frac{\mathcal{A}_{b(\nu)_a}^{\{...,\nu_{k,a}\pm2,...\}}}{\Delta_k}\left(\frac{\partial E_{\text{hom}}}{\partial p_b} - \frac{1}{\beta}\frac{\partial\beta}{\partial p_b}E_{\text{pert},(\nu)} \pm \frac{1}{\beta}\frac{\partial\beta}{\partial p_b}\Delta_k\right)\end{aligned} \tag{8.94}$$

which yields exactly the functions $C_{1/2,(\nu),k}(b, p_b)$ from above and supports the total result. Finally, it is easy to show that the symbol function $\boldsymbol{\pi}_1$ also trivially satisfies (S1–2).

(S2): Construction of the Moyal Unitary $\boldsymbol{u}_{(1)}$

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

$$\boldsymbol{\pi}_{\text{R}} := \sum_{a=1}^{d_{(\nu)}} \zeta_{(\nu)_a} \langle \zeta_{(\nu)_a}, \cdot \rangle_{\mathcal{F}_{\text{s}}}. \tag{8.95}$$

The mediator between $\boldsymbol{\pi}\mathcal{H}_{\text{pert}}$ and $\mathcal{K}_{\text{pert}}$, and vice versa, has the zeroth order component

$$\boldsymbol{u}_0(b) := \sum_{(n)} \zeta_{(n)} \langle \xi_{(n)}(b), \cdot \rangle_{\mathcal{F}_{\text{s}}} \tag{8.96}$$

where the sum over (n) is a sum over all possible combinations of excitation numbers in the field Fock space. It is straightforward to show that $\boldsymbol{u}_0$ and $\boldsymbol{\pi}_{\text{R}}$ together with $\boldsymbol{\pi}_0$ satisfy the base clause of the construction rules (S2), namely (S2–1) $\boldsymbol{u}_0^* \cdot \boldsymbol{u}_0 = \mathbf{1}_{\text{pert}}$, (S2–2) $\boldsymbol{u}_0 \cdot \boldsymbol{u}_0^* = \mathbf{1}_{\text{pert}}$, and (S2–3) $\boldsymbol{u}_0 \cdot \boldsymbol{\pi}_0 \cdot \boldsymbol{u}_0^* = \boldsymbol{\pi}_{\text{R}}$. The hermitian contribution to $\boldsymbol{u}_1$ trivially vanishes because $\boldsymbol{u}_0$ soleley depends on b. The antihermitian part $\boldsymbol{k}_1 \cdot \boldsymbol{u}_0$ is then determined by the equation

$$[\boldsymbol{k}_1, \boldsymbol{\pi}_{\text{R}}]_{\text{pert}} + \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1 \cdot \boldsymbol{u}_0^* = 0 \tag{8.97}$$

with a solution that yields for $\boldsymbol{u}_1$

$$\boldsymbol{u}_1 = [\boldsymbol{\pi}_{\text{R}}, \boldsymbol{u}_0 \cdot \boldsymbol{\pi}_1 \cdot \boldsymbol{u}_0^*]_{\text{pert}} \cdot \boldsymbol{u}_0. \tag{8.98}$$

With $\boldsymbol{\pi}_1$ in equation (8.90), this gives the following result:

$$\begin{aligned} \boldsymbol{u}_1 = \frac{i}{2} \sum_{a=1}^{d_{(\nu)}} \sum_{k \in \Sigma} \Big(& \mathcal{A}_{b(\nu)_a}^{\{..,\nu_{k,a}-2,..\}} C_{1,(\nu),k} \left(\zeta_{(\nu)_a} \langle \xi_{\{..,\nu_{k,a}-2,..\}}, \cdot \rangle_{\mathcal{F}_{\text{s}}} + \zeta_{\{..,\nu_{k,a}-2,..\}} \langle \xi_{(\nu)_a}, \cdot \rangle_{\mathcal{F}_{\text{s}}} \right) \\ & + \mathcal{A}_{b(\nu)_a}^{\{..,\nu_{k,a}+2,..\}} C_{2,(\nu),k} \left(\zeta_{(\nu)_a} \langle \xi_{\{..,\nu_{k,a}+2,..\}}, \cdot \rangle_{\mathcal{F}_{\text{s}}} + \zeta_{\{..,\nu_{k,a}+2,..\}} \langle \xi_{(\nu)_a}, \cdot \rangle_{\mathcal{F}_{\text{s}}} \right) \Big). \end{aligned} \tag{8.99}$$

(S3): Construction of the Effective Hamiltonian $\boldsymbol{h}_{\mathit{eff},(2)}$

According to the rule (S3), i.e., $\boldsymbol{h}_{\text{eff}} = \boldsymbol{u} \star_\varepsilon \boldsymbol{H} \star_\varepsilon \boldsymbol{u}^*$, the scheme yields for the zero order contribution of the restricted effective Hamilton symbol $\boldsymbol{h}_{\text{eff},(2),\text{R}} = \boldsymbol{h}_{\text{eff},0,\text{R}} + \varepsilon \boldsymbol{h}_{\text{eff},1,\text{R}} + \varepsilon^2 \boldsymbol{h}_{\text{eff},2,\text{R}}$, the following result:

$$\begin{aligned} \boldsymbol{h}_{\text{eff},0,\text{R}}(b, p_b) &:= \boldsymbol{\pi}_{\text{R}} \cdot \boldsymbol{u}_0 \cdot \boldsymbol{H}_0 \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\text{R}} \\ &= \Big(-\frac{1}{12} \beta \frac{p_b^2}{b^2} + \tilde{\Lambda} \beta^3 \Big) \boldsymbol{\pi}_{\text{R}} + \frac{1}{\beta} \sum_{a=1}^{d_{(\nu)}} \sum_{k \in \Sigma} \omega(b, k^2)\, \nu_{k,a}\, \zeta_{(\nu)_a} \langle \zeta_{(\nu)_a}, \cdot \rangle_{\mathcal{F}_{\text{s}}}. \end{aligned} \tag{8.100}$$

This corresponds to the Born–Oppenheimer adiabatic limit of the perturbation theory in which the effective Hamiltonian for the gravitational degrees of freedom not only contains the first "bare" gravitational homogeneous part $E_{\text{hom}}(b, p_b)$ but also the backreaction contribution from the Klein–Gordon energy band (ν). Starting with the first order contribution, we obtain according

to equation (6.212)

$$\boldsymbol{h}_{\text{eff},1} = \left(\boldsymbol{u}_1 \cdot \boldsymbol{H}_0 - \boldsymbol{h}_{\text{eff},0} \cdot \boldsymbol{u}_1 + \frac{i}{2}\{\boldsymbol{u}_0, \boldsymbol{H}_0\}_{\text{hom}} - \frac{i}{2}\{\boldsymbol{h}_{\text{eff},0}, \boldsymbol{u}_0\}_{\text{hom}}\right) \cdot \boldsymbol{u}_0^*. \tag{8.101}$$

Recall that $\boldsymbol{u}_1$ has no diagonal contributions according to (8.99), and that $\boldsymbol{u}_0$ is independent of p_b. Therefore, $\boldsymbol{h}_{\text{eff},1}$ has no diagonal contributions at all such that $\boldsymbol{h}_{\text{eff},1,\text{R}} := \boldsymbol{\pi}_\text{R} \cdot \boldsymbol{h}_{\text{eff},1} \cdot \boldsymbol{\pi}_\text{R}$ vanishes identically. Recall that $\boldsymbol{h}_{\text{eff},2,\text{R}}$ is given by

$$\boldsymbol{h}_{\text{eff},2,\text{R}} = \boldsymbol{\pi}_\text{R} \cdot \left(\frac{i}{2} \left(\{\boldsymbol{u}_1, \boldsymbol{H}_0 + E_{(\nu)}\, \mathbf{1}_{\text{pert}}\}_{\text{hom}} - \{\boldsymbol{h}_{\text{eff},1}, \boldsymbol{u}_0\}_{\text{hom}} \right) - \boldsymbol{h}_{\text{eff},1} \cdot \boldsymbol{u}_1 \right) \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_\text{R}. \tag{8.102}$$

Note that $\boldsymbol{h}_{\text{eff},1}$ is non–vanishing, in constrast to $\boldsymbol{h}_{\text{eff},1,\text{R}}$, and its non–vanishing contributions need to be taken into account in the evaluation of $\boldsymbol{h}_{\text{eff},2,\text{R}}$. However, we have already shown that $\boldsymbol{\pi}_\text{R} \cdot \boldsymbol{h}_{\text{eff},1} = 0$ due to symmetry reasons. By pulling the symbol $\boldsymbol{\pi}_\text{R}$ into the Poisson bracket of the second term, which is allowed since $\boldsymbol{\pi}_\text{R}$ is independent of b and p_b, also the second term vanishes. Thus, the evaluation of $\boldsymbol{h}_{\text{eff},2,\text{R}}$ is confined to the first contribution. Using the result for $\boldsymbol{u}_1$ in equation (8.99) yields *a priori* for the second order contribution of the effective Hamilton symbol

$$\begin{aligned}\boldsymbol{h}_{\text{eff},2,\text{R}} = \sum_{a=1}^{d_{(\nu)}} \left(\sum_{k\in\Sigma} \left(\frac{C_{3,(\nu)}}{\omega_k^3} \left(\nu_{k,a} + \frac{1}{2} \right) + \frac{C_{4,(\nu)}}{\omega_k^4} \left(\nu_{k,a}^2 + \nu_{k,a} + 1 \right) + \frac{C_{5,(\nu)}}{\omega_k^5} \left(\nu_{k,a} + \frac{1}{2} \right) \right) \right) \\ \cdot \zeta_{(\nu)_a} \langle \zeta_{(\nu)_a}, \cdot \rangle_{\mathcal{F}_\text{s}},\end{aligned} \tag{8.103}$$

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

$$C_{3,(\nu)}(b, p_b) := \frac{\mu^4 b^2}{8} \left(\frac{1}{\beta^3} \left(\frac{\partial \beta}{\partial p_b} \right)^2 - \frac{1}{\beta^2} \left(\frac{\partial^2 \beta}{\partial p_b^2} \right) \right) = -\frac{\sigma^2 \mu^4 b^2}{8\,\beta^5}, \tag{8.104}$$

$$C_{4,(\nu)}(b, p_b) := \frac{\mu^4 b^2}{16} \left(\frac{2}{\beta} \frac{\partial \beta}{\partial p_b} \frac{\partial E_{\text{hom}}}{\partial p_b} + \frac{\partial^2 E_{\text{hom}}}{\partial p_b^2} - \frac{1}{\beta} \frac{\partial^2 \beta}{\partial p_b^2} E_{\text{pert},(\nu)} \right), \tag{8.105}$$

$$C_{5,(\nu)} := \frac{\mu^4 b^2}{8} \left(2 \frac{\partial \beta}{\partial p_b} \frac{\partial E_{\text{hom}}}{\partial p_b} E_{\text{pert},(\nu)} - \beta \left(\frac{\partial E_{\text{hom}}}{\partial p_b} \right)^2 - \frac{1}{\beta} \left(\frac{\partial \beta}{\partial p_b} \right)^2 E_{\text{pert},(\nu)}^2 \right). \tag{8.106}$$

Note that these functions do not depend on the wave vector k which has been employed as a summation index in (8.103). They act as multiplicative functions which could be pulled out of the sums. We emphasize that this result can easily be obtained by using and extending the explicit results in terms of the connection coefficients used for the oscillator and the cosmological toy models. The explicit evaluation of the energy functions shows that several terms include higher orders in the perturbation parameter ε. In particular, it is clear from the definitions (8.71) that σ is proportional to ε, and hence the terms including derivatives of $\beta = \sqrt{b^2 + \sigma^2 \frac{p_b^2}{b^2}}$ with respect to p_b contribute additional factors of ε. One can do this straightforward computation and show

that the only remaining terms at second order are

$$\boldsymbol{h}_{\mathrm{eff},2,\mathrm{R}}|_2 = -\frac{3\,\mu^4}{32}\sum_{a=1}^{d_\nu}\zeta_{(\nu)_a}\langle\zeta_{(\nu)_a},\cdot\,\rangle_{\mathcal{F}_\mathrm{s}} \cdot\sum_{k\in\Sigma}\left(\frac{b^4}{\Sigma^3}\frac{1}{\omega(k^2)^4}\left(\nu_{k,a}^2+\nu_{k,a}+1\right)+\frac{3\,p_b^2b^2}{\beta}\frac{1}{\omega(k^2)^5}\left(\nu_{k,a}+\frac{1}{2}\right)\right). \tag{8.107}$$

We emphasize that the sums over all modes k in (8.107) converge. First, the integers $\nu_{k,a}$ are only non–vanishing for a finite number of modes k which solves the convergence problem for terms which enter with polynomials of $\nu_{k,a}$. The remaining constant contributions however benefit from the high inverse order of $\omega(b,k^2)=\sqrt{k^2+\mu^2b^2}$ that enters. It is thus possible to explicitely compute the effective Hamilton symbol up to second order in ε for the cosmological field model and we obtain a convergent result despite the mode sums. The next aim would be to find solutions with respect to the non–trivial slow scalar part of $\boldsymbol{h}_{\mathrm{eff},(2),\mathrm{R}}$. The application of the operator $\hat{\boldsymbol{u}}$ then yields wave functions in $\mathcal{H}$ which are exact solutions up to errors of order ε^3. We leave this task to future research, and emphasize that techniques to solve the Hamiltonian problem similar to the one for the homogeneous cosmological toy model will be necessary.

9. Gauge–Invariant Inhomogeneous Cosmology

9.1. Gauge–Invariant Cosmological Perturbations

In this chapter, we apply SAPT to inhomogeneous quantum cosmological perturbation theory with gauge–invariant perturbation variables. The scheme proceeds in a similar manner as in the previous chapter but is, in contrast, completely constrained. The goal is to compute the backreaction from the inhomogeneous perturbations exerted on the homogeneous degrees of freedom. The chapter mainly relies on (Schander and Thiemann 2019c) which serves as a basis for sections 9.1 and 9.3 in which we apply the SAPT scheme to two inhomogeneous cosmological models and prepare this application accordingly. Sections 9.2 and 9.4 are based on the more general considerations in (Schander and Thiemann 2019a).

9.1.1. Cosmological Perturbation Theory

The model rests on a four–dimensional globally hyperbolic space time manifold $\mathcal{M} \cong \mathbb{R} \times \sigma$. The gravitational field g on $\mathcal{M}$ is, as usual, a two–times covariant, symmetric, and non–degenerate tensor field with signature $(-,+,+,+)$. The spatial hypersurfaces σ are compact and flat three–tori $\sigma \cong \mathbb{T}^3$ with side lenghts $l \equiv 1$. As the matter content, we consider again a real–valued Klein–Gordon scalar field Φ. We adopt a $(3+1)$–split of space time as developed by Arnowitt, Deser, and Misner (1959) (see section 2.1.1). Due to the global hyperbolicity, $\mathcal{M}$ foliates into Cauchy surfaces Σ_t parametrized by a global time function t. n^μ is the unit normal vector field to these hypersurfaces, N and $\mathcal{N}_\mu$ the (standard) lapse and shift functions which parametrize the normal and the tangential part of the foliation. The spatial metric on $\mathbb{T}^3$ induced by g is defined as $h_{\mu\nu} := g_{\mu\nu} + n_\mu n_\nu$. The associated extrinsic curvature is given by $K_{\mu\nu} = h^\rho_\mu h^\lambda_\nu \nabla_\rho n_\lambda$. ∇ is the unique torsion–free covariant derivative associated to the metric g. After pulling back the tensor fields to $\mathbb{T}^3$ and denoting spatial indices on the spatial hypersurfaces with lower case latin symbols $a, b, c, .. \in \{1,2,3\}$, the Lagrange density is expressed by the sum of the Einstein–Hilbert Lagrange density $\mathcal{L}_{\mathrm{EH}}$ and the scalar field Lagrange density $\mathcal{L}_\Phi$ with

$$\mathcal{L}_{\mathrm{EH}} = \frac{1}{2\kappa}\sqrt{|h|}N\left(R^{(3)} + K_{ab}K^{ab} - (K^a_a)^2 - 2\Lambda\right), \tag{9.1}$$

$$\mathcal{L}_\Phi = \frac{1}{2\lambda}\sqrt{|h|}N\left(-\frac{1}{N^2}\dot{\Phi}^2 + 2\frac{\mathcal{N}^a}{N^2}\dot{\Phi}\partial_a\Phi + \left(h^{ab} - \frac{\mathcal{N}^a\mathcal{N}^b}{N^2}\right)\partial_a\Phi\partial_b\Phi + m^2\Phi^2\right). \tag{9.2}$$

We recall that $\kappa = 8\pi G = {M_{\mathrm{Pl}}}^{-2}$ is the gravitational coupling constant, $\lambda \in \mathbb{R}^+$ is the coupling constant of the scalar field, $m \in \mathbb{R}^+$ is the mass parameter of the scalar field, and $R^{(3)}$ is the curvature scalar associated with the three–metric h and its Levi–Civita covariant derivative D. The only degrees of freedom of the spatially homogeneous and isotropic sector are the zeroth

order lapse function $N_0(t)$ which is a Lagrange multiplier, and the scale factor a associated with the zeroth order spatial metric $h^0(t,x) := a^2(t)\tilde{h}^0(x)$ with $\tilde{h}^0(x)$ being the time–independent metric on the spatial hypersurfaces (cf. section 2.2). For the flat three–torus $\tilde{h}^0$ is simply the Euclidean spatial metric restricted to the respective domain. Its determinant evaluates to one.

We introduce perturbations of the homogeneous degrees of freedom using a decomposition into scalar, vector and tensor parts according to their properties regarding $SO(3)$–transformations. A detailed analysis of cosmological perturbation theory within the Hamiltonian framework for closed FLRW universes was initiated and performed by Halliwell and Hawking (1987). Since we make use of their results in a later stage, we will stick to the definition of perturbations used by Castelló Gomar, Martín-Benito, and Mena Marugán (2015) and Martínez and Olmedo (2016), and which is given by

$$N(t,x) =: N_0(t) + a^3(t)\,\eta(t,x) \tag{9.3}$$

$$\mathcal{N}_a(t,x) =: a^2(t)\,D_a\,k(t,x) + a^2(t)\,\epsilon_a^{\ bc} D_b\,k_c(t,x) \tag{9.4}$$

$$\begin{aligned} h_{ab}(t,x) =: a^2(t)\Big[&(1+2\,\alpha(t,x))\,\tilde{h}^0_{ab}(x) + 6\Big(D_aD_b - \frac{1}{3}\tilde{h}^0_{ab}(x)D_cD^c\Big)\beta(t,x) \\ &+ 2\sqrt{6}\,t_{ab}(t,x) + 4\sqrt{3}D_{(a}v_{b)}(t,x)\Big], \end{aligned} \tag{9.5}$$

$$\Phi(t,x) =: \phi(t) + \varphi(t,x). \tag{9.6}$$

The homogeneous and isotropic degrees of freedom (N_0, a, ϕ) are functions of the time parameter t while the inhomogeneous fields $\eta, k, \alpha, \beta, \varphi, v_a, k_a, t_{ab}$ depend on both the time variable and the spatial degrees of freedom x. We denote the perturbative scalar fields by $(\eta, k, \alpha, \beta, \varphi)$, the vector degrees of freedom by v_a and k_a, and the tensor field perturbations by t_{ab}. For notational reasons, we introduce the fields $\check{k} := \Delta k$ and $\check{k}_a := \epsilon_a^{\ bc} D_b k_c$ as new degrees of freedom associated with the shift.

9.1.2. Legendre Transformation

We insert the perturbed variables from equations (9.3) – (9.6) into the Lagrange density in (9.1) and (9.2), and expand the Lagrangian and the action functional S up to second order in the perturbations. As the three–torus does not have a boundary, total divergences vanish in the computations. The resulting action does neither depend on the velocities of the lapse variables N_0 and η, nor on the velocities of the shift variables $\check{k}$ and $\check{k}_a$. This implies that lapse and shift are Lagrange multipliers and will hence be associated to primary constraint equations in the Hamiltonian formalism. We perform a Legendre transformation in the lines of Castelló Gomar, Martín-Benito, and Mena Marugán (2015) and Halliwell and Hawking (1987), and define the conjugate momenta (P_a, P_ϕ) for the homogeneous and isotropic degrees of freedom (a, ϕ) using the Lagrange function $L = \int \mathrm{d}x\,\mathcal{L}$ which gives

$$P_a := \frac{\partial L}{\partial \dot{a}} = -\frac{6}{\kappa N} a\dot{a}, \qquad P_\phi := \frac{\partial L}{\partial \dot{\phi}} = \frac{a^3}{\lambda N}\dot{\phi}. \tag{9.7}$$

We denote the corresponding phase space by $\Gamma_{\mathrm{hom}} = \Gamma_{\mathrm{s}}$. The perturbation fields $(\alpha, \beta, \varphi, v_a, t_{ab})$ together with their conjugate momenta $(\pi_\alpha, \pi_\beta, \pi_\varphi, \pi_v^a, \pi_t^{ab})$ span the perturbative phase space

$\Gamma_{\text{pert}} = \Gamma_{\text{f}}$. The perturbative momenta are defined according to

$$\pi_\chi := \frac{\partial \mathcal{L}}{\partial \dot{\chi}} \tag{9.8}$$

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

$$\begin{aligned}\mathcal{H} = N_0 \left[\mathcal{H}_0 + \mathcal{H}_2^{\text{s}} + \mathcal{H}_2^{v} + \mathcal{H}_2^{t}\right] + \eta \cdot \mathcal{H}_1^{\eta} + \check{k}_a \cdot \mathcal{H}_1^{\check{k}_d,a} + \check{k} \cdot \mathcal{H}_1^{\check{k}} \\ + \lambda_{N_0} \cdot \Pi_0^{N_0} + \lambda_\eta \cdot \Pi_1^{\eta} + \lambda_{\check{k}} \cdot \Pi_1^{\check{k}} + \lambda_{\check{k}_a,b} \cdot \Pi_1^{\check{k}_a,b}.\end{aligned} \tag{9.9}$$

$\mathcal{H}_0$ denotes the zeroth order Hamiltonian contribution associated with the completely homogeneous and isotropic model. $\mathcal{H}_2^{\text{s}}$, $\mathcal{H}_2^{v}$ and $\mathcal{H}_2^{t}$ are of second order in the perturbations and contain only scalar, vector and tensor variables respectively. $\mathcal{H}_1^{\eta}$, $\mathcal{H}_1^{\check{k}_d,a}$ and $\mathcal{H}_1^{\check{k}}$ represent first order contributions which factorize with the respective lapse and shift variables. The second line lists the primary constraints associated with lapse and shift and their Lagrange multipliers λ_{N_0}, λ_η, $\lambda_{\check{k}}$ and $\lambda_{\check{k}_a,b}$. As it turns out, the system is completely constrained and we thus perform a Dirac analysis to extract the relevant physics. We refer to chapter 2 for an overview of the Dirac constraint analysis.

Identifying Suitable Variables

The constraint analysis can be performed most easily by first identifying a suitable set of free variables – in fact, it will then become a trivial task. We start by noting that the perturbation variables that we introduced are not all gauge–invariant. In the scalar sector, it is convenient to introduce the gauge–invariant Mukhanov-Sasaki variable ϑ (Mukhanov 1988, 2005) given by

$$\vartheta := a\,\varphi + \frac{6\lambda P_\phi}{\kappa P_a}(\alpha - \Delta\beta). \tag{9.10}$$

Note that this transformation for the perturbative fields also depends on the homogeneous degrees of freedom. While the original perturbation variables had canonical momenta properly defined by the Legendre transform, the mapping to new perturbation variables will break the canonical structure as it depends very non–trivially on the homogeneous degrees of freedom. In order to preserve the canonical structure of the system, it is mandatory to find a suitable transformation for the homogeneous and isotropic variables, too. This appears to be a cumbersome mission. Castelló Gomar, Martín-Benito, and Mena Marugán (2015) have however shown that it is possible to find a transformation for the homogeneous and isotropic degrees of freedom which preserves the canonical structure of the system up to second order in the cosmological scalar perturbations.

While identifying the most suitable degrees of freedom which will preserve the canonical structure up to second order in the cosmological perturbation, we should also be concerned with the closure of the constraint algebra. In general, the algorithm might entail a large number of constraints that are needed to guarantee consistency of the dynamics. The idea, put forward by Castelló Gomar, Martín-Benito, and Mena Marugán (2015) and Martínez and Olmedo (2016) is to use some of the secondary constraints of the Dirac algorithm as the canonical variables them-

selves. Thereby, the Dirac algorithm becomes partly trivial just by implementing the first set of secondary constraints. In summary, the aim of the following procedure is then threefold.

Firstly, we introduce gauge–invariant variables for the perturbations in order to allow for a generic choice of variables, and not to be a restricted to a specific choice of coordinates. Secondly, we aim at keeping the canonical structure of the theory, at least up to second order in the cosmological perturbations. For the latter purpose, we will review the Dirac algorithm for constrained systems and implement additional transformations for the homogeneous and isotropic degrees of freedom. In particular, we modify the homogeneous variables by adding second order contributions in the cosmological perturbations. Thirdly, we wish to construct a theory whose dynamics will be unitarily implementable at the quantum level. Therefore, we consider further canonical transformations with respect to the perturbations. Their effects on the homogeneous variables will be taken into account accordingly.

Following the work by Castelló Gomar, Martín-Benito, and Mena Marugán (2015) and by Martínez and Olmedo (2016), the formalism proceeds as follows: As a starting point, we consider the homogeneous and isotropic degrees of freedom as non–dynamical background variables. This offers the possibility to introduce perturbation variables which build a canonical set with respect to the dynamical perturbative system only.

New Variables in the Tensor Sector

We start with the canonical pair of the tensor perturbations (t_{ab}, π_t^{ab}) which is already gauge–invariant by construction. In this respect, no transformation is necessary that would possibly break the canonical structure of the entire system. However, we would like to work with classical perturbation variables whose dynamics is unitarily implementable in the quantum theory. This simply amounts to eliminating contributions in the Hamiltonian which couple the perturbation variables with their respective momenta. In this way, the final Hamiltonian at second order will only consist of terms proportional to squares of the perturbation variables or squares of the perturbation momenta after a suitable transformation. In other words, after a Fourier transformation, the Hamiltonian has the form of a sum of harmonic oscillators with masses and frequencies that possibly depend on the homogeneous and isotropic degrees of freedom. Indeed, these transformations guarantee the unitarity of the perturbation's quantum dynamics when considered in a semiclassical framework of a QFT on CST. Martínez and Olmedo (2016) suggest an appropriate transformation for the tensor perturbations, which however, breaks the canonical structure. They consequently perform an additional transformation of the homogeneous degrees of freedom. This transformation supplements the original variables by second order perturbative contributions. Following their procedure, we denote the shifted, new homogeneous variables by $(\check{a}, \check{P}_a, \check{\phi}, \check{P}_\phi)$.

Implementing these new variables in the Hamilton constraint, the transformations yield additional terms in the Hamiltonian which are of second order in the tensor perturbations. We absorb these terms in $\mathcal{H}_2^t$ and denote the new tensor Hamiltonian as $\check{\mathcal{H}}_2^t$. Furthermore, the transformations result into a shift of the lapse function by second order contributions which will be taken into account by a function denoted as $\check{N}_2$.

New Variables in the Vector Sector

Regarding the vector perturbations, we can identify the constraints $\mathcal{H}_1^{\check{k}_d,a}$ and their conjugate variables $C_{1,a}^{\check{k}_d} := 2\sqrt{3}\,v_a$ as canonical pairs. This choice is ideally suited in order to obtain a preferably simple constraint algebra at the end. It entails an additional transformation for the homogeneous degrees of freedom in order to preserve the (almost) canonical structure, similar the the procedure for the tensor perturbations. The new variables, which also include the transformations from the tensor perturbations, shall be denoted by $(\grave{a}, \grave{P}_a, \grave{\phi}, \grave{P}_\phi)$. The transformations result in a new second order vectorial part of the Hamiltonian $\grave{\mathcal{H}}_2^{\vartheta}$ which is proportional to the constraint $\mathcal{H}_1^{\check{k}_d,a}$ itself. Note that we also express the linear constraint $\mathcal{H}_1^{\check{k}_d,a}$ in terms of the new variables. However, the form of the constraint does not change since we cut after the second perturbative order and the new homogeneous variables only differ by contributions in second order. Thus, if we demand that $\mathcal{H}_1^{\check{k}_d,a}$ vanishes as a constraint, this implies that $\grave{\mathcal{H}}_2^{v}$ vanishes automatically. Hence, there is no vector constraint contributing to the second order Hamilton constraint as long as the first order constraint is satisfied which means that its solution is trivial and we have no longer to include it into our considerations.

New Variables in the Scalar Sector

In the scalar sector, we employ the Mukhanov–Sasaki scalar field ϑ as introduced above. Castelló Gomar, Martín-Benito, and Mena Marugán (2015) suggest to consider the first order constraints $\mathcal{H}_1^{\eta}$ and $\mathcal{H}_1^{\check{k}}$ as the remaining new scalar perturbation variables. Since these constraints do not commute with respect to the perturbative Poisson brackets, we shift $\mathcal{H}_1^{\eta}$ by a linear term in the perturbations and we denote the new constraint variable by $\bar{\mathcal{H}}_1^{\eta}$. The latter Poisson commutes with $\mathcal{H}_1^{\check{k}}$ if for the time being we only consider the perturbations as dynamical degrees of freedom. This procedure entails another shift of the lapse function which yields the new lapse function $\bar{N}_2$ emanating from $\check{N}_2$. In a next step, we construct the conjugate variables with respect to the *inhomogeneous* Poisson brackets denoting them by π_v, C_1^{η} and $C_1^{\check{k}}$. The new canonical pairs in the scalar sector of the perturbations are thus $(\vartheta, \pi_\vartheta)$, $(C_1^{\eta}, \bar{\mathcal{H}}_1^{\eta})$ and $(C_1^{\check{k}}, \mathcal{H}_1^{\check{k}})$. Finally, we complete the transformation in the homogeneous sector by adding second order contributions to the initial homogeneous canonical pairs. This yields the new variables $(\tilde{a}, \tilde{P}_a, \tilde{\phi}, \tilde{P}_\phi)$ in the homogeneous sector. The implementation of the transformations yields new contributions to $\mathcal{H}$: Some of them include only the Mukhanov–Sasaki canonical variables and we correspondingly absorb them into a new second order scalar Hamiltonian $\tilde{\mathcal{H}}_2^{s}$. Another contribution is proportional to the zeroth order Hamiltonian $\mathcal{H}_0$ such that it is possible to absorb them into $\bar{N}_2$ which becomes $\check{N}_2$. In addition, the transformations result into new second order contributions which are proportional to the linear constraints $\bar{\mathcal{H}}_1^{\eta}$ and $\mathcal{H}_1^{\check{k}}$. We denote these contributions as G_1 and K_1 respectively.

In total, the transformations result in the following Hamiltonian density

$$\begin{aligned}\tilde{\mathcal{H}} = &\left(N_0 + \check{N}_2\right)\cdot\left[\mathcal{H}_0 + \tilde{\mathcal{H}}_2^{s} + \grave{\mathcal{H}}_2^{v} + \check{\mathcal{H}}_2^{t}\right] + (\eta + G_1)\cdot\bar{\mathcal{H}}_1^{\eta} + \left(\tilde{k} + K_1\right)\cdot\mathcal{H}_1^{\check{k}} + \check{k}_a\cdot\mathcal{H}_1^{\check{k}_d,a}\\ &+ \lambda_{N_0}\cdot\Pi_0^{N_0} + \lambda_\eta\cdot\Pi_1^{\eta} + \lambda_{\check{k}}\cdot\Pi_1^{\check{k}} + \lambda_{\check{k}_b,a}\cdot\Pi_1^{\check{k}_b,a}.\end{aligned} \tag{9.11}$$

We emphasize that the constraint $\tilde{\mathcal{H}}$ is to be expressed in terms of the new homogeneous variables

$(\tilde{a}, \tilde{P}_a, \tilde{\phi}, \tilde{P}_\phi)$ which finally amounts to simply replacing non–dashed variables by the dashed ones as we cut after the second order in perturbations. The second line in equation (9.11) accounts for the set of primary constraints $(\Pi_0^{N_0}, \Pi_1^\eta, \Pi_1^{\check{k}}, \Pi_1^{\check{k}_b,a})$ with their respective Lagrange multipliers $(\lambda_{N_0}, \lambda_\eta, \lambda_{\check{k}}, \lambda_{\check{k}_b,a})$. These primary constraints already appeared in equation (9.9) and have remained unchanged under the preceding transformations.

9.1.3. Dirac Constraint Analysis

We are now ready to perform the Dirac constraint analysis based on the new variables and constraints emanating from the previous transformations. We first consider the primary constraints which imply that the system restricts to the submanifold of the phase space defined by

$$\Pi_0^{N_0} = 0, \quad \Pi_1^\eta = 0, \quad \Pi_1^{\check{k}} = 0, \quad \Pi_1^{\check{k}_b,a} = 0. \tag{9.12}$$

Consequently, the associated Lagrange multipliers λ_{N_0}, λ_g, $\lambda_{\check{k}}$ and $\lambda_{\check{k}_b,a}$ can be chosen arbitrarily. In a second step, consistency of the dynamics requires that the primary constraints are preseverd (i.e., remain zero) under the evolution generated by the full Hamilton constraint $\tilde{\mathcal{H}}$. This requirement gives rise to the secondary constraints

$$\left\{\tilde{\mathcal{H}}, \Pi_0^{N_0}\right\} = \mathcal{H}_0 + \tilde{\mathcal{H}}_2^s + \grave{\mathcal{H}}_2^v + \check{\mathcal{H}}_2^t \approx 0, \tag{9.13}$$

$$\left\{\tilde{\mathcal{H}}, \Pi_1^\eta\right\} = \bar{\mathcal{H}}_1^\eta \approx 0, \tag{9.14}$$

$$\left\{\tilde{\mathcal{H}}, \Pi_1^{\check{k}}\right\} = \mathcal{H}_1^{\check{k}} \approx 0, \tag{9.15}$$

$$\left\{\tilde{\mathcal{H}}, \Pi_1^{\check{k}_b,a}\right\} = \mathcal{H}_1^{\check{k}_b,a} \approx 0 \tag{9.16}$$

where "≈ 0" means that the expression on the left hand side must vanish at least weakly, i.e., on the primary constraint surface. Note that now, the Poisson brackets include the dynamics with respect to *all* canonical pairs of the transformed system both the homogeneous and the inhomogeneous ones.

The next step consists in checking whether the secondary constraints in the equations (9.13) - (9.16) are preserved under the dynamics of $\tilde{\mathcal{H}}$ or if they entail further secondary constraints. The computations are trivial since the preceding transformations imply that the first order constraints $\bar{\mathcal{H}}_1^\eta$, $\mathcal{H}_1^{\check{k}}$ and $\mathcal{H}_1^{\check{k}_d,a}$ are canonical variables, and hence commute with all other variables except with their respective conjugate variables C_1^η, $C_1^{\check{k}}$ and $C_1^{\check{k}_d,a}$. Indeed, C_1^η appears in $\tilde{\mathcal{H}}$ within the first order functions G_1 and K_1, and thus, entails non–vanishing Poisson brackets with $\bar{\mathcal{H}}_1^\eta$. Since these Poisson brackets enter however with an additional constraint factor, they vanish at least weakly, namely

$$\left\{\tilde{\mathcal{H}}, \mathcal{H}_0 + \tilde{\mathcal{H}}_2^s + \grave{\mathcal{H}}_2^v + \check{\mathcal{H}}_2^t\right\} = 0, \tag{9.17}$$

$$\left\{\tilde{\mathcal{H}}, \bar{\mathcal{H}}_1^\eta\right\} = \left\{G_1, \bar{\mathcal{H}}_1^\eta\right\} \bar{\mathcal{H}}_1^\eta + \left\{K_1, \bar{\mathcal{H}}_1^\eta\right\} \mathcal{H}_1^{\check{k}} \approx 0, \tag{9.18}$$

$$\left\{\tilde{\mathcal{H}}, \mathcal{H}_1^{\check{k}}\right\} = \left\{G_1, \mathcal{H}_1^{\check{k}}\right\} \bar{\mathcal{H}}_1^g + \left\{K_1, \mathcal{H}_1^{\check{k}}\right\} \mathcal{H}_1^{\check{k}} = 0. \tag{9.19}$$

Hence, the constraint algebra closes and as a consequence, it suffices to evaluate the primary and

the first set of secondary constraints to solve the system. In particular, we must guarantee that the equations

$$\bar{\mathcal{H}}_1^{\eta} = 0, \qquad \mathcal{H}_1^{\check{k}} = 0, \qquad \mathcal{H}_1^{\check{k}_b,a} = 0, \qquad \mathcal{H}_0 + \tilde{\mathcal{H}}_2^s + \grave{\mathcal{H}}_2^v + \check{\mathcal{H}}_2^t = 0 \tag{9.20}$$

are satisfied on the constraint surface. Since $\bar{\mathcal{H}}_1^{\eta}$, $\mathcal{H}_1^{\check{k}}$ and $\mathcal{H}_1^{\check{k}_b,a}$ were defined as canonical momenta, we can simply impose the first three equations by requiring that these momenta be vanishing. We recall that the second order vector constraint $\grave{\mathcal{H}}_2^v$ is zero whenever $\mathcal{H}_1^{\check{k}_b,a} = 0$ is satisfied.

9.1.4. The Hamilton Constraint

From the previous discussion, it follows that the only non–trivial constraint of the cosmological system is

$$\mathcal{C} := \mathcal{H}_0 + \tilde{\mathcal{H}}_2^s + \check{\mathcal{H}}_2^t = 0. \tag{9.21}$$

As a consquence, the total constraint $C := \int \mathrm{d}x\, \mathcal{C}$ splits into three parts. Omitting the dashes over the transformed homogeneous variables in order to keep the notation simple, these are given by

$$H_0 := -\kappa \frac{P_a^2}{12\tilde{a}} + \frac{\Lambda}{\kappa} a^3 + \frac{\lambda P_\phi^2}{2a^3} + \frac{1}{2\lambda} m^2 a^3 \phi^2, \tag{9.22}$$

$$\tilde{H}_2^s := \frac{1}{2a} \int_{\mathbb{T}^3} \mathrm{d}x \left[\lambda \pi_\vartheta^2 + \vartheta \left[-\frac{\Delta}{\lambda} + M_{\mathrm{MS}}(a, P_a, \phi, P_\phi)^2 \right] \vartheta \right], \tag{9.23}$$

$$\check{H}_2^t := \frac{1}{2a} \int_{\mathbb{T}^3} \mathrm{d}x \left[\frac{\kappa\, \pi_t^{ab} \pi_{t,ab}}{6} + t^{ab} \left[-\frac{3}{\kappa}\Delta + M_{\mathrm{T}}(a, P_a, \phi)^2 \right] t_{ab} \right] \tag{9.24}$$

where we recall that $(\vartheta, \pi_\vartheta, t_{ab}, \pi_t^{ab})$ are inhomogeneous and thus x–dependent fields. $\Delta := D_a D^a$ is the Laplace–Beltrami operator on the three–torus. We defined the Mukhanov–Sasaki mass function $M_{\mathrm{MS}}(a, P_a, \phi, P_\phi)$ and the tensor mass function $M_{\mathrm{T}}(a, P_a, \phi)$ according to

$$M_{\mathrm{MS}}^2 := -\frac{\kappa^2 P_a^2}{18\lambda a^2} + \frac{7\kappa P_\phi^2}{2a^4} - 12\, m^2 \frac{a\phi P_\phi}{\lambda P_a} - 18 \frac{\lambda P_\phi^4}{a^6 P_a^2} + \frac{m^2}{\lambda} a^2, \tag{9.25}$$

$$M_{\mathrm{T}}^2 := \frac{\kappa P_a^2}{6\, a^2} - 3\frac{m^2}{\lambda}\, a^2 \phi^2 - 6\frac{\Lambda}{\lambda} a^2. \tag{9.26}$$

The total Hamiltonian constraint $C = H_0 + \tilde{H}_2^s + \check{H}_2^t$ is the object of interest in the subsequent application of SAPT.

Epsilon–Rescalings

To make contact with SAPT, we rescale the canonical pairs that we obtained by the transformations in the previous section using the dimensionless parameter $\varepsilon^2 := \frac{\kappa}{\lambda}$. In the homogeneous sector, we define

$$p_a := \varepsilon^2 P_a, \qquad p_\phi := \varepsilon P_\phi. \tag{9.27}$$

In the perturbative sector, we rescale the Mukhanov–Sasaki field variables and the tensor field variables according to

$$\breve{\vartheta} := \frac{\vartheta}{\varepsilon}, \quad \breve{\pi}_\vartheta := \varepsilon\,\pi_\vartheta \quad \text{and} \quad \breve{t}_{ab} := \frac{t_{ab}}{\varepsilon^2}, \quad \breve{\pi}_t^{ab} := \varepsilon^2\,\pi_t^{ab}. \tag{9.28}$$

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

$$H_0 = -\frac{p_a^2}{12a} + \frac{p_\phi^2}{2a^3} + \frac{1}{2}\varepsilon^2 m^2 a^3\phi^2 + \Lambda a^3, \tag{9.29}$$

$$\tilde{H}_2^s = \frac{1}{2a}\int_{\mathbb{T}^3} \mathrm{d}x\, \left(\pi_\vartheta^2 + \vartheta\,\varepsilon^4\left(-\Delta + M_{\mathrm{MS}}^2\right)\vartheta\right), \tag{9.30}$$

$$\breve{H}_2^t = \frac{1}{2a}\int_{\mathbb{T}^3} \mathrm{d}x\, \left(\frac{\pi_t^{ab}\pi_{t,ab}}{6} + t^{ab}\varepsilon^4\left(-3\Delta + (\varepsilon\,M_{\mathrm{T}})^2\right)t_{ab}\right), \tag{9.31}$$

and for which the mass terms now become according to the definitions (9.25) and (9.26)

$$M_{\mathrm{MS}}^2 = -\frac{p_a^2}{18a^2} + \frac{7p_\phi^2}{2a^4} - 12\varepsilon m^2\frac{a\phi p_\phi}{p_a} - 18\,\frac{p_\phi^4}{a^6 p_a^2} + m^2a^2, \tag{9.32}$$

$$(\varepsilon M_{\mathrm{T}})^2 = \frac{p_a^2}{6a^2} - 3\varepsilon^2 m^2 a^2\phi^2 - 6\Lambda a^2. \tag{9.33}$$

Note that the transformations for the perturbation fields (9.28) are canonical while the canonical structure of the homogeneous degrees of freedom changes due to the rescaling in (9.27).

Quantization

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

$$[\hat{a}, \hat{p}_a]_{\mathrm{hom}} = i\,\varepsilon^2\hat{1}_a, \quad [\hat{\phi}, \hat{p}_\phi]_{\mathrm{hom}} = i\,\varepsilon\hat{1}_\phi \tag{9.34}$$

where the subscript "hom" indicates that the commutator is with respect to the homogeneous quantum algebra. The operators $\hat{1}_a$ and $\hat{1}_\phi$ denote the unity operators in $\mathcal{H}_a$ and $\mathcal{H}_\phi$ respectively. Note that any of the operators is defined on the whole $\mathcal{H}_{\mathrm{hom}}$ but we always omit trivial factors of unity. The space adiabatic perturbation scheme requires us to use a symmetric Weyl quantization prescription which we are going to employ in the following. We note that the scheme considers

the homogeneous and isotropic degrees of freedom as the ones whose canonical structure becomes rescaled by a very small parameter, hence they will be identified as the "slow" variables and be subject to a phase space quantization. We associate the fast sector of the model with the cosmological inhomogeneities, i.e., the Mukhanov–Sasaki and tensor perturbations. In a strict sense, one can however not identify these sectors with a respectively "slow" or "fast" dynamics – there simply is no dynamics since the system is completely constrained.

Bold characters indicate quantum operators of the inhomogeneous system and the quantum fields are given for any time $t \in \mathbb{R}$ by the operator–valued distributions $(\boldsymbol{\vartheta}(t), \boldsymbol{\pi}_\vartheta(t), \boldsymbol{t}_{ab}(t), \boldsymbol{\pi}_t^{ab}(t))$ on $\mathbb{T}^3$. We denote the Hilbert space of the Mukhanov–Sasaki quantum system by $\mathcal{H}_{\mathrm{MS}}$, the tensor Hilbert space as $\mathcal{H}_{\mathrm{T}}$, and the total Hilbert space of the inhomogeneities arises naturally as the tensor product of the two latter as $\mathcal{H}_{\mathrm{pert}} = \mathcal{H}_{\mathrm{MS}} \otimes \mathcal{H}_{\mathrm{T}}$. We employ the standard canonical commutation relations for the perturbation fields. Therefore, we introduce two contravariant test tensor fields $f(x)$ and $F_{ab}(x)$ of rank 0 and 2 respectively as well as two covariant test tensor fields $j(x)$ and $J^{ab}(x)$ of rank 0 and 2 respectively. The quantum commutation relations consequently have the form

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

where the subscript "pert" indicates that the commutator is with respect to operators on the perturbative Hilbert space $\mathcal{H}_{\mathrm{pert}}$, and $\mathbf{1}_{\mathrm{MS}}$ and $\mathbf{1}_{\mathrm{T}}$ denote the unity operators on the respective Mukhanov–Sasaki and tensor subspaces. Again, we omit any trivial factor of unity. With this, we are ready to quantize the Hamilton constraint C as a whole. Therefore, we carefully split its contributions in equations (9.29) – (9.33) into its homogeneous and inhomogeneous contributions, quantize these parts respectively and glue them together with tensor products (just as we did for the dust model). This yields the formal expression

$$\hat{\boldsymbol{C}} = \hat{\boldsymbol{H}}_0 + \hat{\boldsymbol{H}}_2^{\mathrm{s}} + \hat{\boldsymbol{H}}_2^{\mathrm{t}} \tag{9.35}$$

which is of course of little direct interest as exact solutions are out of reach. Instead, we employ SAPT and consider the known phase space quantization scheme for the homogeneous sector.

Partial Phase Space Quantization

Following SAPT, we quantize the Hamilton function with respect to the inhomogeneous sector only and obtain the Hamilton constraint symbol $\boldsymbol{C}$ given by

$$\boldsymbol{C} = H_0\,\mathbf{1}_{\mathrm{pert}} + \tilde{\boldsymbol{H}}_2^{\mathrm{s}} + \check{\boldsymbol{H}}_2^{\mathrm{t}} \tag{9.36}$$

with $\mathbf{1}_{\mathrm{pert}} = \mathbf{1}_{\mathrm{MS}} \otimes \mathbf{1}_{\mathrm{T}}$ and using the expressions (9.29) – (9.31). As before, it is most useful to employ annihilation and creation operators. Although not mandatory, let us consider the basis states $f_k(x) = \exp(ikx)$ of the one–particle Hilbert space $\mathcal{H}_{\mathbb{T}^3} = L^2(\mathbb{T}^3, \mathrm{d}x)$ where $k \in \Bbbk := 2\pi\mathbb{Z}^3 \setminus \{0\}$. The Hilbert spaces of the perturbative quantum field theories are then given by the symmetric Fock spaces $\mathcal{F}_{\mathrm{s}}(\mathcal{H}_{\mathbb{T}^3})$ associated with the one–particle Hilbert space. More precisely, the total perturbative Hilbert space comprises the symmetric Mukhanov–Sasaki Fock space $\mathcal{F}_{\mathrm{s,MS}}$ as well as two symmetric Fock spaces associated with the tensor degrees of freedom. Indeed, the tensor

field carries only two independent degrees of freedom corresponding to the two polarizations of the tensor modes. These will be labeled by the index $\tau = \{+, -\}$ and we write for the Fock spaces $\mathcal{F}_{\mathrm{s,T},\pm}$. The total Hilbert space is given as the tensor product

$$\mathcal{H}_{\mathrm{pert}} = \mathcal{F}_{\mathrm{s,MS}}(\mathcal{H}_{\mathbb{T}^3}) \bigotimes_{\tau=\{+,-\}} \mathcal{F}_{\mathrm{s,T},\tau}(\mathcal{H}_{\mathbb{T}^3}). \tag{9.37}$$

We define the one–particle frequency operators for the Mukhanov–Sasaki and the tensor system by

$$\omega_{\mathrm{MS}} := \varepsilon^2\sqrt{-\Delta + M_{\mathrm{MS}}^2}, \quad \omega_{\mathrm{T}} := \varepsilon^2\sqrt{-18\Delta + 6\,(\varepsilon\, M_{\mathrm{T}})^2}. \tag{9.38}$$

Note that both operators depend on the homogeneous degrees of freedom as they contain the mass functions $M_{\mathrm{MS}}(a, p_a, \phi, p_\phi)$ and $M_{\mathrm{T}}(a, p_a, \phi)$. To avoid confusion with the scale factor variable, we will denote the annihilation and creation operators of the Mukhanov–Sasaki system with the symbols $\boldsymbol{b}$ and $\boldsymbol{b}^*$. They arise using an (a, p_a, ϕ, p_ϕ)–dependent representation map $\pi_{(a,p_a,\phi,p_\phi)} : \mathcal{A}_Q \to \mathcal{L}(\mathcal{H}_{\mathrm{pert}})$ from the field Weyl algebra $\mathcal{A}_Q$ to the space of linear operators on Fock space. As operator–valued distributions on the space of smearing functions $C_0^\infty(\mathbb{T}^3)$, they are given for any $f \in C_0^\infty(\mathbb{T}^3)$ by

$$\boldsymbol{b}(f) := \frac{1}{\sqrt{2}}\,\pi\left[\big(\sqrt{\omega_{\mathrm{MS}}}\boldsymbol{\vartheta}\big)(f) - i\big(\sqrt{\omega_{\mathrm{MS}}}^{-1}\boldsymbol{\pi}_\vartheta\big)(f)\right], \tag{9.39}$$

and they explicitely depend on the slow phase space variables through the frequency ω_{MS}. The creation operator $\boldsymbol{b}^*(f)$ arises from $\boldsymbol{b}(f)$ by taking its adjoint. Likewise, one defines annihilation and creation operators $\boldsymbol{d}_\pm(f)$ and $\boldsymbol{d}_\pm^*(f)$ for the two tensor modes by replacing ω_{MS} by ω_{T} and by replacing the fields $(\boldsymbol{\vartheta}, \boldsymbol{\pi}_\vartheta)$ by the two pairs of tensorial fields which we denote by $(\boldsymbol{t}_\pm, \boldsymbol{\pi}_{t,\pm})$. For fixed homogeneous variables (a, p_a, ϕ, p_ϕ), the commutation relations for the Mukhanov–Sasaki field evaluate to

$$[\boldsymbol{b}(f_1), \boldsymbol{b}^*(f_2)]_{\mathrm{pert}} = \langle f_1, f_2\rangle\, \mathbf{1}_{\mathrm{MS}} \tag{9.40}$$

where $f_1, f_2 \in C_0^\infty(\mathbb{T}^3)$, and likewise for the graviton fields.

It will prove useful to pass to a mode representation and in the following we refer to the annihilation and creation operators of a mode $k \in \mathbb{k}$ for the Mukhanov–Sasaki system by $\boldsymbol{b}_k$ and $\boldsymbol{b}_k^*$. For the tensor modes, we define the set of vectors $K \in \mathbb{K} := \{\mathbb{k}, \tau\}$ with $\tau \in \{-, +\}$ to denote the annihilation and creation operators by $\boldsymbol{d}_K$ and $\boldsymbol{d}_K^*$. The commutation relations have the form

$$\big[\boldsymbol{b}_k, \boldsymbol{b}_{k'}^*\big]_{\mathrm{pert}} = \delta_{k,k'}\mathbf{1}_{\mathrm{MS}}, \quad \big[\boldsymbol{d}_K, \boldsymbol{d}_{K'}^*\big]_{\mathrm{pert}} = \delta_{K,K'}\mathbf{1}_{\mathrm{T}}, \tag{9.41}$$

and the δ's are Kronecker deltas since we are on the compact three–torus. Since the f_k's are eigenfunctions of the Laplace–Beltrami operator, we have that $(\Delta f_k)(x) = -k^2 f_k(x)$, and it is possible to label the frequency operators accordingly by $\omega_{\mathrm{MS}}(k^2)$ and $\omega_{\mathrm{T}}(k^2)$ when evaluated on f_k. It is then straightforward to express the normal–ordered Hamilton constraint symbol function $\boldsymbol{C} \in C^\infty(\Gamma_{\mathrm{s}}, \mathcal{L}(\mathcal{H}_{\mathrm{pert}}))$ by means of the creation and annihilation operators and the associated frequency functions

$$\boldsymbol{C} = E_{\mathrm{hom}}(a, p_a, \phi, p_\phi)\,\mathbf{1}_{\mathrm{pert}} + \frac{1}{a}\sum_{k\in\mathbb{k}} \omega_{\mathrm{MS}}(k^2)\,\boldsymbol{b}_k^*\,\boldsymbol{b}_k + \frac{1}{6a}\sum_{K\in\mathbb{K}} \omega_{\mathrm{T}}(k^2)\,\boldsymbol{d}_K^*\,\boldsymbol{d}_K \tag{9.42}$$

where we conveniently denoted the purely homogeneous Hamilton function from equation (9.29) by E_{hom} and omitted trivial factors of unity. We emphasize that not only the zeroth order offset energy contribution E_{hom} depends on the homogeneous phase space variables but also the frequency functions $\omega_{\mathrm{MS}}(k^2)$ and $\omega_{\mathrm{T}}(k^2)$ as well as any of the annihilation and creation operators of the Mukhanov–Sasaki and tensor systems.

9.1.5. Checking of the Conditions

In order to see whether SAPT applies to the presented model, we go through the conditions (C1) – (C4). Regarding condition (C1), the total Hilbert space has the form of the tensor product

$$\mathcal{H} = \mathcal{H}_{\mathrm{hom}} \otimes \mathcal{H}_{\mathrm{pert}} \tag{9.43}$$

where the second factor identifies with the perturbative Fock Hilbert spaces while the first is given by the homogeneous space of states. Note that this was only achievable because of the almost canonical transformations that we performed in section 9.1.1. As a consequence, we can unitarily relate the states induced by different Fock representations.

To continue with the remaining conditions, let us assume for the time being that $\boldsymbol{C}$ is a physical Hamilton operator, and we are interested in its entire spectrum. From equation (9.42), it is easy to deduce that $\boldsymbol{C}$ admits a discrete spectrum for any fixed $(a, p_a, \phi, p_\phi) \in \Gamma_{\mathrm{hom}}$ because the sums over the (generalized) wave vectors in the Hamilton constraint are discrete and so is the spectrum of the number operators $\boldsymbol{b}_k^* \boldsymbol{b}_k$ and $\boldsymbol{d}_K^* \boldsymbol{d}_K$ when applied to vectors in the total Fock space $\mathcal{H}_{\mathrm{pert}}$. Any Fock state $\xi_{(n)} \in \mathcal{H}_{\mathrm{pert}}$ with finite energy identifies with a finite set of non–vanishing quantum numbers $(n) := \{\dots, n_{\mathrm{MS},k_1}, n_{\mathrm{MS},k_2}, \dots, n_{\mathrm{T},\tau,k_1}, n_{\mathrm{T},\tau,k_2}, \dots\}$ where we distinguished between the quantum numbers of the Mukhanov–Sasaki and the tensor perturbations, and $k_1, k_2, \dots$ run over $2\pi\mathbb{Z}^3$. We also introduce degeneracy labels which take the possibility of degenerate eigenstates into account, and we denote them by $b = 1, \dots, d$ for the Mukhanov–Sasaki system and by $b' = 1, \dots, d'$ for the graviton system. To shorten the notation, we integrate the degeneracy labels in $\beta := \{b, b'\}$ and the degeneracy numbers in $\delta := \{d, d'\}$. According to equation (9.42), the discrete eigenvalue problem for any finite set of quantum numbers $(n)_\beta$ then has the form

$$\begin{aligned} \boldsymbol{C}(a, p_a, \phi, p_\phi)\, \xi_{(n)_\beta}(a, p_a, \phi, p_\phi) &= E_{(n)}(a, p_a, \phi, p_\phi)\, \xi_{(n)_\beta}(a, p_a, \phi, p_\phi), \\ E_{(n)}(a, p_a, \phi, p_\phi) &:= E_{\mathrm{hom}}(a, p_a, \phi, p_\phi) + \frac{1}{a} \sum_{k \in \mathbb{k}} n_{\mathrm{MS},k,b}\, \omega_{\mathrm{MS}}(k^2) + \frac{1}{6a} \sum_{K \in \mathbb{K}} n_{\mathrm{T},K,b'}\, \omega_{\mathrm{T}}(k^2). \end{aligned} \tag{9.44}$$

To further shorten the notation, we write for the set of homogeneous phase space variables $(q, p) := (a, p_a, \phi, p_\phi)$. The eigenvalue problem in $\mathcal{H}_{\mathrm{pert}}$ is then given by

$$\boldsymbol{C}(q, p)\, \xi_{(n)_\beta}(q, p) = E_{(n)}(q, p)\, \xi_{(n)_\beta}(q, p). \tag{9.45}$$

Due to the discreteness of the eigenbasis, it is possible to define non–vanishing energy gaps between the eigenenergy bands of the perturbations at least for local regions in phase space. In the following, we assume that the relevant energy bands admit such local gaps in the region of interest.

Now, condition (C2) requires that the quantum Hamilton constraint $\hat{\boldsymbol{C}}$ is given as the Weyl quantization of the symbol function $\boldsymbol{C}(a, p_a, \phi, p_\phi)$ which is implemented by definition. Furthermore, $\boldsymbol{C}$ should have values in the space of bounded self–adjoint operators on $\mathcal{H}_{\text{pert}}$, should be a bounded function with respect to a and ϕ and maximally admit a polynomial growth with respect to the momenta p_a and p_ϕ. Obviously, $\boldsymbol{C}(a, p_a, \phi, p_\phi)$ is neither a (polynomially) bounded function with respect to the homogeneous variables nor is it a bounded operator on the inhomogeneous Fock spaces and which would be required to satisfy (C2). In order to satisfy condition (C2) and to secure convergence of the perturbation series for the problem at hand, it would be necessary to define an auxiliary Hamiltonian symbol $\boldsymbol{C}_{\text{aux}}$ that satisfies (C2) and which generates approximately the same dynamics as the original Hamiltonian (see chapter 6). However, this is not achievable without further ado since $\boldsymbol{C}(a, p_a, \phi, p_\phi)$ is an unbounded operator. Again, we are left with two choices: We either define an operator $\boldsymbol{C}_{\text{aux}}$ that satisfies (C2) but which will not entirely reflect the properties of $\boldsymbol{C}$ or we retain the original Hamilton constraint at the cost of obtaining possibly non–convergent adiabatic perturbation theories. We remain here with the second option, and stress that convergence (e.g., with respect to a weak operator topology) of the perturbative series for the first option would need to be investigated by independent means.

Let us also note that both the homogeneous and the inhomogeneous contributions to the constraint $\boldsymbol{C}(a, p_a, \phi, p_\phi)$ depend on ε, either via E_{hom} or via $\omega_{\text{MS}}(k^2)$ and $\omega_{\text{T}}(k^2)$. Following SAPT, these different contributions in ε should be split in a power series expansion with respect to ε such that several non–vanishing power series coefficients in ε can be identified and be treated at different orders of the SAPT scheme. Here however, we will subsume the whole constraint $\boldsymbol{C}$ under its zeroth order contribution $\boldsymbol{C}_0$ in order to simplify the task of applying SAPT. This procedure does not change the final result as long as one carefully sorts the contributions *after* the application of SAPT. Since this section should rather be seen as a first explorative investigation of SAPT for gauge–invariant cosmological perturbation theory, we will defer from performing this analysis and simply set $\boldsymbol{C} \equiv \boldsymbol{C}_0$.

Regarding condition (C3), we note once again that due to the discreteness of the modes k and K certain regions in the homogeneous phase space can be identified where no eigenvalue crossings occur. We will assume that we can restrict our investigations to such a region in phase space.

Finally, condition (C4) assures the convergence of the results but we have already stated that condition (C2) can not be met without further ado, and which prohibits any results on the convergence of the perturbative series. We will hence not be able to make any further statements regarding convergence here but as mentioned before SAPT can be applied regardless.

9.1.6. Analysis of the Perturbation Eigenfunctions

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

$$\xi_{(\nu)}(q, p) = \prod_{k\in\mathbb{k}} \prod_{K\in\mathbb{K}} \frac{(\boldsymbol{b}_k^*)^{\nu_{\text{MS},k}}}{\sqrt{\nu_{\text{MS},k}!}} \frac{(\boldsymbol{d}_K^*)^{\nu_{\text{T},K}}}{\sqrt{\nu_{\text{T},K}!}}\, \Omega(q, p). \tag{9.46}$$

We introduce the explicit representation of the Mukhanov–Sasaki wave function and the tensor wave functions as a product by

$$\xi_{(n)} =: \xi^{\mathrm{MS}}_{(\nu_{\mathrm{MS}})} \cdot \prod_{\tau} \xi^{\mathrm{T},\tau}_{(\nu_{\mathrm{T}})}. \tag{9.47}$$

Recall that the creation and annihilation operators for the Mukhanov–Sasaki and the graviton modes (see equation (9.39)) depend explicitely on the homogeneous phase space variables through the masses within the frequency functions

$$\omega_{\mathrm{MS}}(q,p,k^2) = \varepsilon^2\sqrt{k^2 + M^2_{\mathrm{MS}}(q,p)}, \quad \omega_{\mathrm{T}}(q,p,k^2) = \varepsilon^2\sqrt{18k^2 + 6(\varepsilon M_{\mathrm{T}})^2(q,p)}. \tag{9.48}$$

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

$$\frac{\partial \boldsymbol{b}_k(q,p)}{\partial\lambda} := \alpha^{\mathrm{MS}}_{\lambda,k}(q,p)\,\boldsymbol{b}^*_k(q,p) = -\frac{1}{8}\frac{\varepsilon^4\,\partial_\lambda M^2_{\mathrm{MS}}(q,p)}{\omega^2_{\mathrm{MS}}(q,p,k^2)}\,\boldsymbol{b}^*_k(q,p), \tag{9.49}$$

$$\frac{\partial \boldsymbol{d}_K(q,p)}{\partial\lambda} := \alpha^{\mathrm{T}}_{\lambda,K}(q,p)\,\boldsymbol{d}^*_K(q,p) = -\frac{3}{4}\frac{\varepsilon^6\,\partial_\lambda M^2_{\mathrm{T}}(q,p)}{\omega^2_{\mathrm{T}}(q,p,k^2)}\,\boldsymbol{d}^*_K(q,p) \tag{9.50}$$

where we implicitely defined the functions $\alpha^{\mathrm{MS}}_{\lambda,k}$ and $\alpha^{\mathrm{T}}_{\lambda,K}$ in close analogy to the finite dimensional models before and the infinite dimensional dust model. The vacuum state $\Omega(q,p) \in \mathcal{H}_{\mathrm{pert}}$ is defined such that $(\boldsymbol{b}_k\,\Omega)(q,p) = 0$ and $(\boldsymbol{d}_K\,\Omega)(q,p) = 0$ for every $k \in \mathbb{k}$ and every $K \in \mathbb{K}$. These equations, together with the derivatives of the annihilation and creation operators, give rise to a formula for the λ–derivative of the vacuum state given by

$$\frac{\partial\Omega(q,p)}{\partial\lambda} = \sum_{k\in\mathbb{k}} \alpha^{\mathrm{MS}}_{\lambda,k}(q,p)(\boldsymbol{b}^*_k\,\boldsymbol{b}^*_k\,\Omega)(q,p) + \sum_{K\in\mathbb{K}} \alpha^{\mathrm{T}}_{\lambda,K}(q,p)(\boldsymbol{d}^*_K\,\boldsymbol{d}^*_K\,\Omega)(q,p). \tag{9.51}$$

With this, it is straightforward to compute the λ–derivative of any excited state $\xi_{(n)}$ using that $\xi_{(n)}$ can be expressed by application of an appropriate number of creation operators on the vacuum state, see equation (9.46). Again, we define the derivative of the eigenstates with respect to the homogeneous parameters as an application of a connection $\boldsymbol{\mathcal{A}}_\lambda \in C^\infty(\Gamma_{\mathrm{hom}}, \mathcal{L}(\mathcal{H}_{\mathrm{pert}}))$ on the global Hilbert bundle H, and we write

$$\frac{\partial\,\xi_{(n)}(q,p)}{\partial\lambda} =: \boldsymbol{\mathcal{A}}_\lambda\,\xi_{(n)} =: \mathcal{A}_{\lambda(n)}{}^{(m)}\,\xi_{(m)}, \quad \mathcal{A}_{\lambda(n)}{}^{(m)}(q,p) \in C^\infty(\Gamma_{\mathrm{hom}},\mathbb{R})\ \forall(n),(m) \tag{9.52}$$

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

that link the state (n) and the state $\{\dots, n_{\mathrm{MS/T},k} \pm 2, \dots\}$ as

$$\mathcal{A}_{\lambda n_{\mathrm{MS},k}}^{\;\;n_{\mathrm{MS},k}-2}(q,p) := -\alpha^{\mathrm{MS}}_{\lambda,k}(q,p)\sqrt{(n_{\mathrm{MS},k}-1)\cdot n_{\mathrm{MS},k}}, \tag{9.53}$$

$$\mathcal{A}_{\lambda n_{\mathrm{MS},k}}^{\;\;n_{\mathrm{MS},k}+2}(q,p) := \alpha^{\mathrm{MS}}_{\lambda,k}(q,p)\sqrt{(n_{\mathrm{MS},k}+1)\cdot(n_{\mathrm{MS},k}+2)}, \tag{9.54}$$

$$\mathcal{A}_{\lambda n_{\mathrm{T},K}}^{\;\;n_{\mathrm{T},K}-2}(q,p) := -\alpha^{\mathrm{T}}_{\lambda,K}(q,p)\sqrt{(n_{\mathrm{T},K}-1)\cdot n_{\mathrm{T},K}}, \tag{9.55}$$

$$\mathcal{A}_{\lambda n_{\mathrm{T},K}}^{\;\;n_{\mathrm{T},K}+2}(q,p) := \alpha^{\mathrm{T}}_{\lambda,K}(q,p)\sqrt{(n_{\mathrm{T},K}+1)\cdot(n_{\mathrm{T},K}+2)}. \tag{9.56}$$

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

$$\begin{aligned}\frac{\partial\xi_{(n)}(q,p)}{\partial\lambda} = \sum_{k\in\Bbbk}\Big(\mathcal{A}_{\lambda n_{\mathrm{MS},k}}^{\;\;n_{\mathrm{MS},k}-2}\xi^{\mathrm{MS}}_{\{\dots,n_{\mathrm{MS},k}-2,\dots\}} + \mathcal{A}_{\lambda n_{\mathrm{MS},k}}^{\;\;n_{\mathrm{MS},k}+2}\xi^{\mathrm{MS}}_{\{\dots,n_{\mathrm{MS},k}+2,\dots\}}\Big)\prod_{\tau}\xi^{\mathrm{T},\tau}_{(n_{\mathrm{T}})} \\ + \xi^{\mathrm{MS}}_{(n_{\mathrm{MS}})}\prod_{\tau}\sum_{k\in\Bbbk}\Big(\mathcal{A}_{\lambda n_{\mathrm{T},K}}^{\;\;n_{\mathrm{T},K}-2}\xi^{\mathrm{T},\tau}_{\{\dots,n_{\mathrm{T},k}-2,\dots\}} + \mathcal{A}_{\lambda n_{\mathrm{T},K}}^{\;\;n_{\mathrm{T},K}+2}\xi^{\mathrm{T},\tau}_{\{\dots,n_{\mathrm{T},k}+2,\dots\}}\Big)\xi^{\mathrm{T},\tau'\neq\tau}_{(n_{\mathrm{T}})}.\end{aligned} \tag{9.57}$$

9.1.7. Space Adiabatic Construction Scheme

The construction of the space adiabatic symbols is subject to two different perturbative scalings, namely with respect to ε for the homogeneous scalar field, and with respect to ε^2 for the homogeneous gravitational degrees of freedom. As a consequence, the Moyal product for two operator–valued functions $\boldsymbol{A}(q,p), \boldsymbol{B}(q,p) \in S^m_\rho(\Gamma_{\mathrm{hom}}, \mathcal{B}(\mathcal{H}_{\mathrm{pert}}))$ takes the form

$$(\boldsymbol{A}\star_\varepsilon\boldsymbol{B})(q,p) \asymp \left[\boldsymbol{A}\exp\left(\frac{i\varepsilon}{2}\left(\overleftarrow{\partial}_\phi\overrightarrow{\partial}_{p_\phi} - \overleftarrow{\partial}_{p_\phi}\overrightarrow{\partial}_\phi\right) - \frac{i\varepsilon^2}{2}\left(\overleftarrow{\partial}_a\overrightarrow{\partial}_{p_a} - \overleftarrow{\partial}_{p_a}\overrightarrow{\partial}_a\right)\right)\boldsymbol{B}\right](q,p) \tag{9.58}$$

where the vectors indicate the direction in which the partial derivatives act. As we will see in the following, the Moyal product with respect to the gravitational degrees of freedom does not contribute to the computations up to second order in the perturbation scheme. Up to the two different scalings, the scheme proceeds in the lines of chapter 6 and 8.

Construction of the Moyal Projector

The first goal is to compute a Moyal projector symbol up to first order in the perturbations and subject to the split $\boldsymbol{\pi}_{(1)} = \boldsymbol{\pi}_0 + \varepsilon\boldsymbol{\pi}_1$. We choose the discrete eigenstate $\xi_{(\nu)_\beta}(q,p) \in \mathcal{H}_{\mathrm{pert}}$ with quantum number $(\nu)_\beta$ associated with the Hamilton symbol $\boldsymbol{C}(q,p)$ to define

$$\boldsymbol{\pi}_0(q,p) := \sum_\beta \xi_{(\nu)_\beta}(q,p)\,\langle\xi_{(\nu)_\beta}(q,p),\cdot\,\rangle_{\mathcal{F}_{\mathrm{s}}} \tag{9.59}$$

where β denotes again the degeneracy label for the considered state. To determine the first order contribution $\boldsymbol{\pi}_1$, the scheme splits it into a diagonal and an off–diagonal part. As we know from the previous models, the diagonal part is not going to vanish trivially here because the states depend on *both* the homogeneous variables *and* their conjugate momenta. However, the diagonal contribution will not enter the computation for the effective Hamilton symbol and so we leave its computation aside, and directly come to the off–diagonal part $\boldsymbol{\pi}_1^{\mathrm{OD}}$. Following the results from

section 6.7, this symbol is given by

$$\boldsymbol{\pi}_1^{\mathrm{OD}} = \frac{i}{2}\sum_{\beta=1}^{\delta}\sum_{(n)\neq(\nu)_\beta}\frac{A_{(\nu)_\beta(n)}}{E_{(\nu)_\beta}-E_{(n)}}\left(\xi_{(\nu)_\beta}\langle\xi_{(n)},\cdot\rangle_{\mathcal{F}_{\mathrm{s}}}-\xi_{(n)}\langle\xi_{(\nu)_\beta},\cdot\rangle_{\mathcal{F}_{\mathrm{s}}}\right), \tag{9.60}$$

and the function $A_{(\nu)_\beta(n)}(q,p)$ is given in line with the definition in equation (6.134) by

$$\begin{aligned}A_{(\nu)_\beta(n)} = {}& \mathcal{A}_{\phi(\nu)_\beta}^{\ \ (n)}\frac{\partial(E_{(n)}+E_{(\nu)_\beta})}{\partial p_\phi} - \mathcal{A}_{p_\phi(\nu)_\beta}^{\ \ (n)}\frac{\partial(E_{(n)}+E_{(\nu)_\beta})}{\partial\phi}\\ &+(E_{(n)}-E_{(m)})\left(\mathcal{A}_{p_\phi(\nu)_\beta}^{\ \ (m)}\mathcal{A}_{\phi(m)}^{\ \ (n)}-\mathcal{A}_{\phi(\nu)_\beta}^{\ \ (m)}\mathcal{A}_{p_\phi(m)}^{\ \ (n)}\right).\end{aligned} \tag{9.61}$$

Construction of the Moyal Unitary

We construct the unitary symbol up to first order and therefore choose $\mathcal{H}_{\mathrm{pert}}$ as the reference space $\mathcal{K}_{\mathrm{pert}}$. Its basis is determined by fixing a set of numbers $(q_0,p_0)\in\Gamma_{\mathrm{hom}}$ and defining $\{\zeta_{(n)} := \xi_{(n)}(q_0,p_0)\}_{(n)}$ as the natural basis of $\mathcal{K}_{\mathrm{pert}}$. Then, we define the zeroth order contribution to the Moyal unitary to be

$$\boldsymbol{u}_0(q,p) := \sum_{(n)}\zeta_{(n)}\langle\xi_{(n)}(q,p),\cdot\rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{9.62}$$

We also define the reference projection for the relevant energy band according to

$$\boldsymbol{\pi}_{\mathrm{R}} := \sum_{\beta=1}^{\delta}\zeta_{(\nu)_\beta}\langle\zeta_{(\nu)_\beta},\cdot\rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{9.63}$$

We easily verify that the zeroth order conditions for the Moyal unitary are satisfied with these choices. The hermitian part of $\boldsymbol{u}_1(q,p)$ is given in terms of the connection coefficients and the fast eigenstates by

$$\boldsymbol{u}_1^{\mathrm{h}}(q,p) = \sum_{(n),(m),(k)}\left(\mathcal{A}_{\phi(n)}^{\ \ (m)}\mathcal{A}_{p_\phi(m)}^{\ \ (k)}-\mathcal{A}_{p_\phi(n)}^{\ \ (m)}\mathcal{A}_{\phi(m)}^{\ \ (k)}\right)\zeta_{(n)}\langle\zeta_{(k)},\cdot\rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{9.64}$$

Since the sum runs over all possible combinations of quantum numbers, it is clear that the two contributions are equal and cancel each other. We thus have that $\boldsymbol{u}_1^{\mathrm{h}}=0$. The antihermitian part of $\boldsymbol{u}_1$ results then from employing the result for $\boldsymbol{\pi}_1^{\mathrm{OD}}$ in the well–known expression

$$\boldsymbol{u}_1^{\mathrm{ah}} = \left[\boldsymbol{\pi}_{\mathrm{R}},\boldsymbol{u}_0\cdot\boldsymbol{\pi}_1^{\mathrm{OD}}\cdot\boldsymbol{u}_0^*\right]_{\mathrm{pert}}\cdot\boldsymbol{u}_0. \tag{9.65}$$

Construction of the Effective Hamilton Constraint

We evaluate the effective Hamilton constraint symbol according to the third condition $\boldsymbol{h}_{\mathrm{eff}} = \boldsymbol{u}\star_\varepsilon\boldsymbol{C}\star_\varepsilon\boldsymbol{u}^*$, and restrict our interest directly to the reference space, i.e., to $\boldsymbol{h}_{\mathrm{eff,R}} = \boldsymbol{\pi}_{\mathrm{R}}\cdot\boldsymbol{h}_{\mathrm{eff}}\cdot\boldsymbol{\pi}_{\mathrm{R}}$. At

zeroth order, this yields

$$\boldsymbol{h}_{\mathrm{eff},0,\mathrm{R}} = \sum_{b,b'=1}^{d,d'} \left[E_{\mathrm{hom}}(a, p_a, \phi, p_\phi) + \frac{1}{a} \sum_{k\in\mathbb{k}} \nu_{\mathrm{MS},k,b}\, \omega_{\mathrm{MS}}(k^2) + \frac{1}{6a} \sum_{K\in\mathbb{K}} \nu_{\mathrm{T},K,b'}\, \omega_{\mathrm{T}}(k^2) \right] \cdot \zeta_{(\nu)_\beta} \langle \zeta_{(\nu)_\beta}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}} \tag{9.66}$$

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

We stress once again that E_{hom} as well as $\omega_{\mathrm{MS}}(k^2)$ and $\omega_{\mathrm{T}}(k^2)$ depend on ε, and a careful analysis of $\boldsymbol{h}_{\mathrm{eff},0,\mathrm{R}}$ would be necessary to deduct these ε–dependent contributions and to add them to the higher order contributions of the final effective constraint. As mentioned earlier, we will not perform this analysis here.

Coming to the first order contribution to the effective Hamiltonian, we realize (once more) that it vanishes identically as shown in section 6.7.

The second order effective Hamilton symbol includes several contributions but we will show that only one of them is of second order in the perturbative parameter, and hence relevant. First, recall the formulae for determining $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{R}}$ from section 6.7. There are basically three different kinds of contributions. For the first of them, remember that a second order contribution with respect to ε corresponds to a *first* order contribution in the perturbation scheme with respect to the homogeneous gravitational degrees of freedom (a, p_a). Consequently, $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{R}}$ includes the first order effective Hamilton constraint regarding the gravitational ε^2–scheme. However, we already know that the first order effective Hamilton constraint within the relevant energy band vanishes identically and so we can simply drop this term. The other two contributions are due to the ε–scheme with respect to the homogeneous scalar matter field. The first of them arises by computing contributions of the first order Moyal product, and the second from second order contributions to the Moyal product, namely

$$\boldsymbol{h}_{\mathrm{eff},2,\mathrm{R}} = \frac{i}{2}\{\boldsymbol{\pi}_{\mathrm{R}} \cdot \boldsymbol{u}_1, \boldsymbol{C} + E_{(\nu)}\, \mathbf{1}_{\mathrm{f}}\}_{\mathrm{hom}} \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\mathrm{R}} + \boldsymbol{\pi}_{\mathrm{R}} \cdot \left[[\boldsymbol{u}_0 \star_\varepsilon \boldsymbol{C}]_2 - [E_{(\nu)} \star_\varepsilon \boldsymbol{u}_0]_2 \right] \cdot \boldsymbol{u}_0^* \cdot \boldsymbol{\pi}_{\mathrm{R}} \tag{9.67}$$

where the Poisson brackets with subscript "hom" denote the standard Poisson brackets on the homogeneous phase space, and the square brackets with subscript 2 mean that the inside is restricted to exactly second order in the perturbative scheme. We have given an explicit expression of this result in terms of the connection coefficients $\boldsymbol{\mathcal{A}}(q, p)$, the energy functions $E_{(n)}(q, p)$ and the composite function $A_{(\nu)n}(q, p)$ in equations (6.134), (6.162) and (6.163) ff. in section 6.7. We will not state them here again but we review their components and select the contributions that effectively enter at second order in the perturbative scheme. The appearance of terms that actually enter at higher orders in ε stems from the fact that the perturbative Mukhanov–Sasaki and graviton contributions to $\boldsymbol{C}$ are by definition of second order in ε. Nevertheless, it was necessary to include them as zeroth order contributions to make the space adiabatic scheme work at the

technical level. This does not undermine the results but a careful analysis of all terms is required.

We recall that the effective, (a, p_a, ϕ, p_ϕ)–dependent masses of the Mukhanov–Sasaki and the graviton systems depend polynomially on ε with different exponents, and so will their derivatives with respect to the homogeneous variables. Most importantly, we find by inspecting their explicit expressions in equations (9.32) and (9.33) that

$$\frac{\partial(\varepsilon M_{\mathrm{T}})^2}{\partial\phi} \propto \varepsilon^2\, a^2\, \phi \sim \varepsilon^2, \qquad \frac{\partial(\varepsilon M_{\mathrm{MS}})^2}{\partial\phi} \propto \varepsilon\, \frac{a\, p_\phi}{p_a} \sim \varepsilon, \tag{9.68}$$

$$\frac{\partial(\varepsilon M_{\mathrm{T}})^2}{\partial p_\phi} = 0, \qquad \frac{\partial(\varepsilon M_{\mathrm{MS}})^2}{\partial p_\phi} \propto \frac{p_\phi}{a^4}, \frac{p_\phi^3}{a^6 p_a^2} \sim 1. \tag{9.69}$$

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

$$\mathcal{A}_{\phi(n)}^{(m)}\Big|_{\mathrm{T}} \propto \frac{\partial_\phi(\varepsilon M_{\mathrm{T}})^2}{18K^2 + 6(\varepsilon M_{\mathrm{T}})^2} \sim \varepsilon^2, \tag{9.70}$$

$$\mathcal{A}_{p_\phi(n)}^{(m)}\Big|_{\mathrm{T}} = 0, \tag{9.71}$$

$$\mathcal{A}_{\phi(n)}^{(m)}\Big|_{\mathrm{MS}} \propto \frac{\partial_\phi M^2_{\mathrm{MS}}}{k^2 + (\varepsilon M_{\mathrm{MS}})^2} \sim \varepsilon, \tag{9.72}$$

$$\mathcal{A}_{p_\phi(n)}^{(m)}\Big|_{\mathrm{MS}} \propto \frac{\partial_{p_\phi} m^2_{\mathrm{MS}}}{k^2 + (\varepsilon M_{\mathrm{MS}})^2} \sim 1 \tag{9.73}$$

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

$$E_{(m)} - E_{(n)} \sim \varepsilon^2 \tag{9.74}$$

$$(E_{(m)} - E_{(n)})^{-1} \sim \varepsilon^{-2} \tag{9.75}$$

$$\partial_\phi E_{\mathrm{hom}} \propto \varepsilon^2\, a^3\, \phi \sim \varepsilon^2, \tag{9.76}$$

$$\partial_{p_\phi} E_{\mathrm{hom}} \propto \frac{p_\phi}{a^3} \sim 1. \tag{9.77}$$

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

$$\boldsymbol{h}_{\mathrm{eff,2,R}} = -\sum_{\beta,(n)} \frac{1}{E_{(\nu)_\beta} - E_{(n)}}\, \mathcal{A}_{\phi(\nu)_\beta}^{(n)}\Big|_{\mathrm{MS}}\, \mathcal{A}_{\phi(n)}^{(\nu)_\beta}\Big|_{\mathrm{MS}} \left(\frac{\partial E_{\mathrm{hom}}}{\partial p_\phi}\right)^2 \zeta_{(\nu)_\beta}\langle\zeta_{(\nu)_\beta}, \cdot\rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{9.78}$$

The sum over all possible excitation numbers (n) reduces to a sum over the wave modes by eval-

uating the connection coefficients. In particular, we have that

$$\sum_{(n)} \frac{\mathcal{A}_{\phi(\nu)_\beta}^{(n)}\Big|_{\mathrm{MS}} \mathcal{A}_{\phi(n)}^{(\nu)_\beta}\Big|_{\mathrm{MS}}}{E_{(\nu)_\beta} - E_{(n)}} \tag{9.79}$$

$$= \sum_{k\in\mathbb{k}} \left(-\frac{a}{2\omega_{\mathrm{MS},b}(k^2)} \left(\mathcal{A}_{\phi\nu_{\mathrm{MS},k,b}}^{\ \nu_{\mathrm{MS},k,b}-2}\right)^2 + \frac{a}{2\omega_{\mathrm{MS},b}(k^2)} \left(\mathcal{A}_{\phi\nu_{\mathrm{MS},k,b}}^{\ \nu_{\mathrm{MS},k,b}+2}\right)^2 \right)$$

$$= \sum_{k\in\mathbb{k}} \frac{a(\alpha_{\phi,k}^{\mathrm{MS}})^2}{2\omega_{\mathrm{MS},b}(k^2)} \left(-(\nu_{\mathrm{MS},k,b}-1)\nu_{\mathrm{MS},k,b} + (\nu_{\mathrm{MS},k,b}+1)(\nu_{\mathrm{MS},k,b}+2)\right)$$

$$= \sum_{k\in\mathbb{k}} \frac{1}{(k^2+M_{\mathrm{MS}})^{5/2}} \left(\nu_{\mathrm{MS},k,b} - \frac{1}{2}\right) \frac{9}{2} \frac{m^4 a^3 p_\phi^2}{p_a^2}. \tag{9.80}$$

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

$$\boldsymbol{h}_{\mathrm{eff},2,\mathrm{R}}(a,p_a,\phi,p_\phi) = -\sum_{b=1}^{d}\sum_{k\in\mathbb{k}} \frac{1}{(k^2+M_{\mathrm{MS}}^2)^{5/2}} \left(\nu_{\mathrm{MS},k,b} + \frac{1}{2}\right) \frac{9}{2} \frac{m^4 p_\phi^4}{a^3 p_a^2}\, \zeta_{(\nu)_b} \langle \zeta_{(\nu)_b}, \cdot \rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{9.81}$$

Before moving to a thorough discussion of this result, let us emphasize once again that M_{MS}^2 and also $\zeta_{(\nu)_b}$ depend on ε and hence, a careful analysis would be required to deduct the resulting higher order contributions in ε in $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{R}}(a,p_a,\phi,p_\phi)$. However, we will not perform this analysis here.

9.1.8. Discussion of the Results

In the previous section, we have computed the effective Hamilton constraint $\boldsymbol{h}_{\mathrm{eff},(2),\mathrm{R}} = \boldsymbol{h}_{\mathrm{eff},0,\mathrm{R}} + \varepsilon^2 \boldsymbol{h}_{\mathrm{eff},2,\mathrm{R}}$ that quantifies the backreaction of the Fock space energy band with quantum number(s) $(\nu)_\beta$ on the homogeneous degrees of freedom. We emphasize that $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{R}}(a,p_a,\phi,p_\phi)$ is a symbol function on the homogeneous phase space with values in the linear operators on $\mathcal{H}_{\mathrm{pert}}$. First, note that we can split the result into two parts, namely the one including the finite number of non–vanishing relevant quantum numbers $\nu_{\mathrm{MS},k,b}$ for different degeneracy labels b, and the contributions which do not depend on these quantum numbers and hence include any summand of the wave vector sum. The first part only has a finite number of contributions. Remember however that the effective Mukhanov–Sasaki mass squared $M_{\mathrm{MS}}^2(a,p_a,\phi,p_\phi)$ is an *indefinite* function on the homogeneous phase space. It can become negative and hence cancel and even surpass the wave number squared in the denominator of the first factor.

Regarding the first case, in particular if a non–positive mass squared cancels the wave number contribution, we observe that for every wave vector $k \in \mathbb{k}$, there is a (possibly non–connected) three–dimensional region $\gamma_k \subset \Gamma_{\mathrm{hom}}$ in the four–dimensional homogeneous phase space for which this single summand diverges. Since the summation over k is discrete, we expect the divergent surfaces to lie discretely in Γ_{s}. For the first part of the effective Hamiltonian, we have a finite number of such surfaces while for the second part, we have a countably infinite number of divergent surfaces. In addition, the global (third) factor in $\boldsymbol{h}_{\mathrm{eff},2,\mathrm{R}}$ diverges in the limits $a \to 0$, $p_a \to 0$ and $p_\phi \to \pm\infty$.

Despite these divergencies, we emphasize that the symbol Hamilton constraint still needs to be Weyl quantized. It might still be possible to find appropriate solutions. Of course, the divergencies narrow the set of admissible quantum states for which $\hat{\boldsymbol{h}}_{\mathrm{eff},2,\mathrm{R}}$ is a well–defined quantum operator . Besides, the absolute value of a negative mass term might be larger than the wave vector squared such that the total Hamilton constraint symbol would have imaginary contributions. Hence, the question arises whether the final effective Hamilton operator of the theory is self–adjoint or allows for self–adjoint extensions. It is therefore more than reasonable to seek for strategies to circumvent these possible problems.

9.2. Indefinite Mass Squared Operators

9.2.1. Possible Solutions

The Mukhanov–Sasaki and graviton mass squared terms of the previous model are not manifestly positive in all regions of the homogeneous phase space. This is due to the various transformations in the homogeneous and in the inhomogeneous sector which are necessary to obtain a well–defined quantum field theory with gauge–invariant perturbation variables. In this section, we present five strategies which aim at avoiding or attenuating the resulting problems. Our discussion here is based and partially taken from (Schander and Thiemann 2019a).

Before, we point out that the transformations and also the presented strategies apply to rather generic second order Hamiltonians. More generally, one may have several matter or geometry species, e.g., scalar, vector, tensor and spinor modes, (Elizaga Navascués, Martin-Benito, and Mena Marugan 2016). We label the different species by the index ι. Then, the transformations from section 8.1 for the case of one single inhomogeneous scalar field and which we denoted by (r, s, t, u) can be generalized to a set of transformations $(r_\iota, s_\iota, t_\iota, u_\iota)$ for every species. Recall that the transformations resulted in additional terms to the homogeneous degrees of freedom (q^j, p_j), $j = 1, \ldots, d$ which we denoted by $(\chi^j_q, \chi_{p,j})$ and which were of second order in the respective perturbative degrees of freedom. Accordingly, we expect additional terms $(\chi^j_{\iota,q}, \chi_{\iota,p,j})$ for every species ι. Since we perturb the homogeneous contribution of the Hamiltonian only linearly in $(\chi^j_{\iota,q}, \chi_{\iota,p,j})$, and because it is allowed to drop the $(\chi^j_{\iota,q}, \chi_{\iota,p,j})$–corrections for the homogeneous variables in the perturbative part of the Hamiltonian as we cut after second order, the different contributions of the species never mix. Accordingly, we can consider the Hamiltonian symbols to be well defined on the corresponding Fock spaces and the Hilbert–Schmidt conditions are solved. However, the mass squared terms $M^2_\iota(q^j, p_j)$ for each of the species may be indefinite.

Adapted Almost–Canonical Transformations

The first, and probably most natural suggestion, is to exploit the full freedom in the transformations $(r_\iota, s_\iota, t_\iota, u_\iota)$ that led to the additional terms in the respective mass squares M^2_ι for every species ι. In the previous section, we directly limited our attention to a restricted subclass of transformations to simplify the task of finding at least one transformation that suffices our needs. We emphasize that there should be a substantial freedom in the choice of these transformations, and the domain of the phase space where the mass squared functions are positive depends on this free-

dom. Thereupon, this region should not be of any physical significance and the generalization of the transformations is hence a physically motivated criterion.

Restriction of the Phase Space

A second approach consists in restricting the classical phase space of the homogeneous degrees of freedom to a subset $\gamma_{M^2\geq 0} \subset \Gamma_{\text{hom}}$ for which $M_\iota(q,p)^2$ is positive for every species ι, i.e., $M_\iota(q,p)^2 \geq 0$ for every $(q,p) \in \gamma_{M^2\geq 0}$ and every ι. Such a restriction can be achieved by defining new variables v_ι for the associated homogeneous variables and by setting $c_\iota^2 v_\iota^2 = M_\iota^2$ where $c_\iota \in \mathbb{R}$ is a suitable constant. We applied this procedure in chapter 8 where we replaced the original homogeneous canonical pair (a, p_a) by the new canonical pair (b, p_b). With the original variables, the effective mass term was given by

$$M(a,p_a)^2 = a^2\left(m^2 - \frac{\Lambda}{2}\right) - \frac{\varepsilon^2}{72}\frac{p_a^2}{a^2} =: \mu^2 a^2 - \mu^2\delta^2\frac{p_a^2}{a^2}, \tag{9.82}$$

which is not manifestly positive. With the new variables it became $M^2(b) = \mu^2 b^2$ where μ^2 was assumed to be positive. The transformation leading to this new set of variables is given by

$$a^2 = b^2 + \delta^2\frac{p_b^2}{b^2}, \quad p_a = a\frac{p_b}{b}. \tag{9.83}$$

Indeed, if (a, p_a) is canonical also (b, p_b) is a canonical pair, as one can easily show as follows:

$$\{p_b, b\}_{\text{hom}} = \frac{1}{2}\left\{\frac{p_b}{b}, b^2\right\}_{\text{hom}} = \frac{1}{2}\left\{\frac{p_b}{b}, b^2 + \delta^2\left(\frac{p_b}{b}\right)^2\right\}_{\text{hom}} = \frac{1}{2}\left\{\frac{p_a}{a}, a^2\right\}_{\text{hom}} = \{p_a, a\}_{\text{hom}} = 1.$$

This transformation leads hence to the desired positive definite mass squared function $M(b)^2$ of the field theory (given that μ^2 is indeed positive). However, the transformation restricts the range of the variables $(a, p_a) \in \mathbb{R}_+ \times \mathbb{R}$ to the set of pairs (a, p_a) with $a^4 \geq \delta^2 p_a^2$. Consequently, the admissible domain of the homogeneous phase space becomes restricted. Besides, as one can easily see by analyzing the new Hamilton function $H(b, p_b)$ in equation (8.73), these transformations substantially worsen the degree of non–polynomiality of $H(b, p_b)$ which can be a serious disadvantage when it comes to quantizing the theory.

This reasoning also applies to higher dimensional phase spaces with several species ι. An especially nice situation occurs when the mass terms M_ι^2 have mutually vanishing Poisson brackets between them. Namely, in this case, it is reasonable to consider them as action variables and determine the corresponding angle variables as their conjugate variables. Unfortunately, this procedure already fails for a set of tensorial and scalar field modes present at the same time. More generally, we may be able to write M_ι^2 in the form

$$M_\iota(q,p)^2 = F_\iota(q,p)^2\, v_\iota(q,p)^2 \tag{9.84}$$

where $F_\iota(q,p)^2$ is a positive function and $v_\iota(q,p)^2$ may still be indefinite for certain species but the v_ι^2 are mutually commuting for all ι for which v_ι^2 is indefinite. Then, apply the action angle prescription to the new variables v_ι^2 and assume that the number of homogeneous variable pairs

is at least as large as the number of indefinite mass squared terms. In the most general case, we solve the equations $v_\iota^2 = v_\iota(q,p)^2$ for some homogeneous momenta $p_\iota = F_\iota(v_\iota, q^\iota, (q^k, p_k))$ where the (q^k, p_k), $k = \iota + 1, \dots, j$ stands for the remaining phase space variables which are not associated with a perturbative species. The variables $(v_\iota, q^\iota, q^k, p_k)$ coordinatize a new phase space with induced symplectic structure. While these variables fail to be canonical coordinates for the system, they are supposed to have full range in some $\mathbb{R}^{2m}$ in contrast to the p_ι. Finally, we must pass to suitable Darboux coordinates and hope that they are global in order that we may apply Weyl quantization.

Restriction to Admissible Modes

The third possibility is to take the indefinite mass terms M_ι^2 seriously as they stand and to allow them to be negative. Accordingly, for certain ranges of the homogeneous variables, the inhomogeneous symbol operator $\boldsymbol{H}_{\text{pert}}(q,p)$ defines a quantum field theory of tachyons. A possibility to deal with the tachyonic instabilty was suggested by Radzikowski (2008). There, the idea is to construct a (q,p)–dependent Fock space $\mathcal{H}_{(q,p)}$ and to allow only those modes corresponding to eigenfunctions f_k of the Δ such that their eigenvalues of the frequency squared operator $\omega(q,p)^2 = -\Delta^2 + M(q,p)^2$ is bigger or equal to zero, i.e., $k^2 + M(q,p)^2 \geq 0$. Accordingly, the smaller $M(q,p)^2$ becomes, the larger the required infrared cut–off on the admissible modes. Specifically, for the example given above, we find that $M(a,p_a)^2$ becomes very negative for $\frac{p_a^2}{a^2} \to \infty$. Note that this term is proportional to $\dot{a}^2$. Hence, for a baryon or radiation dominated Universe, this term certainly diverges at the classical Big Bang.

For SAPT, this has the following consequence. Recall that for a torus of respective side lengths 1 in all directions, the mode numbers k are discrete, more precisely $k \in \Bbbk = 2\pi\mathbb{Z}^3 \setminus \{0\}$. Let $S_\pm \subset \Gamma_{\text{hom}}$ be the subsets of the slow phase space defined by $M(q,p)^2 \geq 0$ and $M(q,p)^2 < 0$ respectively. Let us consider the spectrum of the Hamilton symbol $\boldsymbol{H}_{\text{pert}}(q,p)$. For example, consider the perturbative and quantized contribution to the dust model in chapter 8 in equation (8.69) with the mass term stated in the previous section or the perturbative Mukhanov–Sasaki and graviton Hamilton symbols obtained after quantizing the functions in equations (9.30) and (9.31). Expressed in terms of the corresponding annihilation and creation operators, it is easy to see that the spectral value associated with a mode f_k has the form

$$E_k(q,p) := \sqrt{c\,k^2 + M(q,p)^2} \tag{9.85}$$

where $c \in \mathbb{R}^+$ is one for the dust model and the Mukhanov–Sasaki field and $c = 18$ for the graviton perturbations. For every point $(q,p) \in S_-$, one can define a discrete set of modes $\mathbb{s}(q,p) \subset \Bbbk$ which consists of all modes for which it holds that $ck^2 > |M(q,p)^2|$, i.e., for all modes in $\mathbb{s}(q,p)$ the energy E_k is well–defined and real. We then impose to disregard all modes in $\Bbbk \setminus \mathbb{s}(q,p)$ individually for every $(q,p) \in S_-$ as well as their associated spectral values $E_k(q,p)$. Consequently, also any eigenstate $\xi_{(n)}(q,p)$ that contains an excitation of these respective mode vectors will be neglected. This obviously affects the computation of the Moyal projector $\boldsymbol{\pi}$ and the Moyal unitary $\boldsymbol{u}$ and accordingly the effective Hamiltonian $\boldsymbol{h}_{\text{eff}}$. For example, the symbol $\boldsymbol{u}$ might not be unitary anymore as it relates the mode bases at different points (q,p), but would become a partial isometry. We would declare the energy band values to vanish for certain modes thus violating the gap

condition. Furthermore, the spectral function $(q, p) \to E_k(q, p)$ has a discontinuity at the surface $ck^2 = |M(q, p)^2|$ on phase space. This can be problematic when computing the Moyal products which require to take derivatives with respect to the homogeneous variables. In total, we admit that this leads to major modifications of the space adiabatic scheme.

Modification of the Quantization Scheme

The fourth proposal presented here suggests to modify the Weyl quantization procedure for the homogeneous variables which is part of the space adiabatic perturbation scheme. In particular, the idea is to restrict the phase space integral over the homogeneous degrees of freedom that enters the Weyl quantization to S_+ in an ad hoc manner. This can be achieved by multiplying all symbol functions such as the Hamiltonian $\boldsymbol{H}(q, p)$ with the characteristic function $\chi_{S_+}(q, p)$ of S_+. This is again not differentiable and it would be more appropriate to substitute χ_{S_+} by a smoothed 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_+. Of course, the quantum theory then will depend on that smoothing procedure which introduces ambiguities and technical challenges because the smoothed version of χ_{S_+} is a highly non–polynomial function of q and p.

Decomposition of the Hamilton Symbol

Finally, the fifth suggestion for how to deal with the indefinite mass squared function is to consider a mode decomposition of the inhomogeneous Hamiltonian contribution $\boldsymbol{H}_{\text{pert}}(q, p)$ and to write for $(q, p) \in S_-$, $\boldsymbol{H}_{\text{pert}}(q, p) := \boldsymbol{H}^+_{\text{pert}}(q, p) + \boldsymbol{H}^-_{\text{pert}}(q, p)$ where $\boldsymbol{H}^+_{\text{pert}}(q, p)$ is the contribution from all modes k with $ck^2 \geq |M(q, p)^2|$. Then, $\boldsymbol{H}^+_{\text{pert}}(q, p)$ may be quantized as before, while the quantization of $\boldsymbol{H}^-_{\text{pert}}(q, p)$ represents a finite sum of flipped quantum harmonic oscillators. The difference of this strategy compared to the third method where we performed a mode–cutting, is exactly that we do not discard $\boldsymbol{H}^-_{\text{pert}}$. We notice that the spectrum of a flipped harmonic oscillator is of the absolutely continuous type, cf. for example (Finster and Isidro 2017). Thus, the spectrum of $\boldsymbol{H}^-_{\text{pert}}$ changes drastically when we transit from S_+ to S_- with corresponding consequences for the space adiabatic perturbation scheme. Unfortunately, such a theory would be unstable.

9.3. Gauge–Invariant Model with Positive Mass Squared

In this section, we apply the second strategy from the previous section to the model with gauge–invariant cosmological perturbations. In particular, we are going to restrict the classical phase space of the homogeneous degrees of freedom to a set of points $(q, p) \in \Gamma_{\text{hom}}$ for which both, the effective Mukhanov–Sasaki effective mass squared $M_{\text{MS}}(q, p)^2$ and the effective graviton mass $M_{\text{T}}(q, p)^2$ are manifestly positive. We achieve this by defining two new sets of homogeneous phase space variables which we denote by (b, q'), and (w, u'). This section is based on and partially taken from (Schander and Thiemann 2019c).

9.3.1. Symplectic Embedding

For simplicity, we restrict our considerations to the case of a vanishing scalar field potential and zero cosmological constant, i.e., $m = 0 = \Lambda$. Then, we consider the rescaled homogeneous variables $(a, p_a\, \phi, p_\phi)$ with Poisson brackets $\{a, p_a\} = \varepsilon^2$, and $\{\phi, p_\phi\} = \varepsilon$. Referring to the definition of the Mukhanov–Sasaki and graviton mass squared functions in equations (9.32) and (9.33), the mass squared functions are given here by

$$M^2_{\rm MS} = -\frac{1}{18}\frac{p_a^2}{a^2} + \frac{7\,p_\phi^2}{2\,a^4} - 18\frac{p_\phi^4}{a^2\,p_a^2}, \quad (\varepsilon\, M_{\rm T})^2 = \frac{p_a^2}{6\,a^2}. \tag{9.86}$$

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

$$M^2_{\rm MS} = \frac{18}{a^4 y^2}\,\left(c_+ y^2 - p_\phi^2\right)\left(p_\phi^2 - c_- y^2\right) \quad \text{with } c_\pm^2 = \frac{1}{72}\left(7 \pm \sqrt{33}\right) \in \mathbb{R}. \tag{9.87}$$

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

$$c_+^2 y^2 > p_\phi^2 > c_-^2 y^2. \tag{9.88}$$

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

$$p_\phi =: y\, w \tag{9.89}$$

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

$$w = \frac{p_\phi}{y}, \quad u' := -\,y\,\phi, \tag{9.90}$$

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

$$\varepsilon^2\,\Theta = -\left(a\,{\rm d}p_a + \varepsilon\,\phi\,{\rm d}p_\phi\right) = -\left((\alpha + \varepsilon\,\phi\,w)\,{\rm d}y - \varepsilon\,u'\,{\rm d}w\right). \tag{9.91}$$

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

$$b := \exp(\alpha + \varepsilon\,\phi\,w) = a \cdot \exp\left(\varepsilon\,\frac{\phi\,p_\phi}{a\,p_a}\right). \tag{9.92}$$

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

$$q' = p_a \cdot \exp\left(-\varepsilon \frac{\phi\, p_\phi}{a\, p_a}\right). \tag{9.93}$$

Note also that the following identity holds

$$\varepsilon \frac{\phi\, p_\phi}{a\, p_a} = -\varepsilon \frac{w\, u'}{b\, q'}. \tag{9.94}$$

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

$$a = b \cdot \exp\left(\varepsilon \frac{w\, u'}{b\, q'}\right), \qquad p_a = q' \cdot \exp\left(-\varepsilon \frac{w\, u'}{b\, q'}\right), \tag{9.95}$$

$$\phi = -\frac{u'}{b\, q'}, \qquad p_\phi = b\, q'\, w. \tag{9.96}$$

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

$$E_{\mathrm{hom}} = \frac{(q')^2}{2b} \exp\left(-\varepsilon \frac{w\, u'}{b\, q'}\right)\left(w^2 - \frac{1}{6}\right), \tag{9.97}$$

$$M^2_{\mathrm{MS}} = 18\, \frac{(q')^2}{b^2}\, \exp\left(-4\, \varepsilon \frac{w\, u'}{b\, q'}\right)\left(c_+ - w^2\right)\left(w^2 - c_-\right), \tag{9.98}$$

$$(\varepsilon M_{\mathrm{T}})^2 = \frac{1}{6}\, \frac{(q')^2}{b^2}\, \exp\left(-4\, \varepsilon \frac{w\, u'}{b\, q'}\right). \tag{9.99}$$

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

9.3.2. Space Adiabatic Construction Scheme

We apply SAPT to the inhomogeneous cosmological model with gauge–invariant perturbations and the appropriate transformations as discussed in section 9.1, but employ the new phase space variables (w, u', b, q'). The Hamilton symbol from (9.42) expressed with these new variables takes

the form

$$\boldsymbol{C}(w,u',b,q') = E_{\mathrm{hom}}(w,u',b,q')\,\mathbf{1}_{\mathrm{pert}} + \frac{e^{-\varepsilon\frac{w\,u'}{b\,q'}}}{b}\left(\sum_{k\in\mathbb{k}}\omega_{\mathrm{MS}}(k^2)\,\boldsymbol{b}_k^*\,\boldsymbol{b}_k + \sum_{K\in\mathbb{K}}\frac{\omega_{\mathrm{T}}(k^2)}{6}\,\boldsymbol{d}_K^*\,\boldsymbol{d}_K^*\right) \tag{9.100}$$

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

Since all formal expressions are identical to the ones in section 9.1, we are content to directly present the expression for the effective Hamilton constraint up to second order in the perturbations. As before, we therefore define an operator–valued symbol $\boldsymbol{\pi}_{\mathrm{R}}$ associated with the fast eigensolution(s) $\zeta_{(\nu)_\gamma} := \xi_{(\nu)_\gamma}(w_0,u_0',b_0,q_0') \in \mathcal{H}_{\mathrm{pert}}$ at some fixed phase space point $(w_0,u_0',b_0,q_0') \in \Gamma_{\mathrm{hom}}$. Thereby, we allow for degenerate eigenstates with degeneracy labels $\gamma = (c,c')$ and the degrees of degeneracy $\delta = (d,d')$ for the Mukhanov–Sasaki and the graviton perturbations respectively. At zeroth order, the scheme generates the standard Born–Oppenheimer result that we directly restrict to the relevant subspace associated with $\boldsymbol{\pi}_{\mathrm{R}}$ and obtain

$$\boldsymbol{C}_{\mathrm{eff},0,\mathrm{R}} = \sum_{c,c'=1}^{d,d'}\left(E_{\mathrm{hom}}(w,u',b,q') + \frac{e^{-\varepsilon\frac{wu'}{bq'}}}{b}\left(\sum_{k\in\mathbb{k}}\nu_{\mathrm{MS},k,c}\,\omega_{\mathrm{MS}}(k^2) + \sum_{K\in\mathbb{K}}\nu_{\mathrm{T},K,c'}\,\frac{\omega_{\mathrm{T}}(k^2)}{6}\right)\right) \cdot \zeta_{(\nu)_\gamma}\langle\zeta_{(\nu)_\gamma},\cdot\,\rangle_{\mathcal{F}_{\mathrm{s}}}. \tag{9.101}$$

The first contribution is simply the standard FLRW Hamiltonian constraint. The two remaining contributions correspond to the bare energy of the chosen excitation number (ν) associated with the Mukhanov–Sasaki and the graviton perturbations. At first order of the scheme, the effective Hamilton constraint vanishes. This is because we assumed that the standard Moyal product applies to the given case, and hence the formulae from the previous section can be used. In this case, the first order effective Hamiltonian vanishes identically.

At second order, it is again possible to split the contributions into a part that only contains the bare symbols and their Poisson brackets and a part which involves the second order Moyal product. The symbolic form of the first part evidently remains the same and we only need to replace the Poisson brackets with respect to the old variables by the Poisson brackets with respect to the new variables. We refer to the previous section for the explicit computations. Analogously, it turns out that many contributions are actually of higher order in ε and can thus be omitted for

our choice of truncation. This yields

$$\frac{i}{2}\{\boldsymbol{\pi}_{\mathrm{R}}\cdot\boldsymbol{u}_1,\boldsymbol{C}+E_{(\nu)}\mathbf{1}_{\mathrm{f}}\}\cdot\boldsymbol{u}_0\cdot\boldsymbol{\pi}_{\mathrm{R}}= \tag{9.102}$$
$$-b\exp\!\left(\varepsilon\frac{wu'}{bq'}\right)\sum_{c,c'=1}^{d,d'}\zeta_{(\nu)_\gamma}\langle\zeta_{(\nu)_\gamma},\cdot\rangle_{\mathcal{F}_{\mathrm{s}}}\left(\sum_{k\in\mathbb{k}}\frac{2\,\nu_{\mathrm{MS},k,c}+1}{64\,\omega_{\mathrm{MS}}(k^2)^5}\cdot\left(\frac{\partial M^2_{\mathrm{MS}}}{\partial u'}\frac{E_{\mathrm{hom}}}{\partial w}-\frac{\partial M^2_{\mathrm{MS}}}{\partial w}\frac{\partial E_{\mathrm{hom}}}{\partial u'}\right)^2\right.$$
$$\left.+\sum_{K\in\mathbb{K}}\frac{27}{8}\frac{2\,\nu_{\mathrm{T},K,c'}+1}{\omega_{\mathrm{T}}(k^2)^5}\cdot\left(\frac{\partial(\varepsilon M_{\mathrm{T}})^2}{\partial u'}\frac{\partial E_{\mathrm{hom}}}{\partial w}\right)^2\right).$$

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

A priori, the scheme includes also contributions to the second order effective Hamilton constraint that are due to the second order Moyal product. However, as before it turns out that these contributions are all of higher than second order in ε, and hence are not relevant for our computations. This finally yields the effective Hamiltonian with respect to the transformed variables (b,q,w,u), i.e., without the ε-scaling for the momentum variables. It consists of the zeroth order contribution (9.101), and the second order contribution (9.102). Expressing the latter explicitly as a function of the transformed variables, we obtain

$$\boldsymbol{C}_{\mathrm{eff},(2),\mathrm{R}}=\sum_{c,c'=1}^{d,d'}\zeta_{(\nu)_\gamma}\langle\zeta_{(\nu)_\gamma},\cdot\rangle_{\mathcal{F}_{\mathrm{s}}} \tag{9.103}$$
$$\cdot\left(\frac{1}{2}\frac{\varepsilon^2q^2}{b^2}\exp\!\left(-\frac{w\,u}{b\,q}\right)\left(w^2-\frac{1}{6}\right)\right.$$
$$+\frac{\exp\left(-\frac{w\,u}{b\,q}\right)}{b}\left(\sum_{k\in\mathbb{k}}\sqrt{k^2+M^2_{\mathrm{MS}}}\,\nu_{\mathrm{MS},k,c}+\frac{1}{6}\sum_{K\in\mathbb{K}}\sqrt{18\,k^2+6\,(\varepsilon M_{\mathrm{T}})^2}\,\nu_{\mathrm{T},K,c'}\right)$$
$$\left.+\sum_{k\in\mathbb{k}}\frac{2\,\nu_{\mathrm{MS},k,c}+1}{(k^2+M^2_{\mathrm{MS}})^{5/2}}\,h_{\mathrm{MS}}(w,u,b,q)+\sum_{K\in\mathbb{K}}\frac{2\,\nu_{\mathrm{T},K,c'}+1}{(18\,k^2+6\,(\varepsilon M_{\mathrm{T}})^2)^{5/2}}\,h_{\mathrm{T}}(w,u,b,q)\right)$$

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

$$h_{\mathrm{MS}}(w,u,b,q)=\exp\!\left(-13\,\frac{w\,u}{b\,q}\right)\left(-\frac{81\,\varepsilon^{12}\,q^6\,w^4}{64\,b^7}\right) \tag{9.104}$$
$$\cdot\left(2\,c_+\,w^2+c_-\left(-8\,c_++2\,w^2+1\right)+c_++4\,w^4-2\,w^2\right)^2,$$
$$h_{\mathrm{T}}(w,u,b,q)=-\exp\!\left(-13\,\frac{w\,u}{b\,q}\right)\cdot\frac{3\,\varepsilon^{12}\,q^6w^4}{2\,b^7}. \tag{9.105}$$

Again, we identify the standard purely homogeneous and isotropic Hamilton constraint of our cosmological model in the first line of this result. Together with the bare energy band contributions from the Mukhanov–Sasaki and tensor perturbations in the ensuing line, this yields the

zeroth order contribution of our perturbative scheme. The last line shows the second order contributions of the scheme. These depend partly on the relevant excitation numbers that we have chosen but there are also contributions which do not, and hence present a vacuum backreaction from the perturbative degrees of freedom on the homogeneous degrees of freedom. Note that effectively, after having performed a transformation to the unscaled momenta (u, q), they both enter with a factor ε^{12}, and terms containing polynomials of them should thus remain very smale within our perturbative scheme. We emphasize once again that we do not expect the same results as for the previous model without the transformations in the homogeneous sector. Another reason for this to happen is that the restriction to the positive mass region is accomplished by a symplectic embedding rather than a symplectomorphism which in particular changes the entire topology of the slow phase space. Thus, the quantum theories cannot be unitarily equivalent. Note that even if the phase spaces were the same and the transformation was strictly canonical, the Moyal products do not simply get rewritten in terms of the new variables unless the canonical transformation is of a restricted type called "gauge equivalent" as defined in the paper by Blaszak and Domanski (2013).

9.3.3. Modifications of the Weyl Quantization Procedure

In the previous section, we performed a symplectic embedding of the homogeneous degrees of freedom that included a restriction of one of the new variables to a union of two compact intervals on the real line. The standard Weyl quantization procedure is however defined for systems with the cotangent bundle over the real line (or products thereof) as their phase space, and hence, the Weyl quantization procedure is a priori not available for this model. In particular, the Moyal product underlying the SAPT scheme might be subject to modifications which would consequently alter the results obtained so far.

If we adhere to the above choice of phase space variables, the definition of the Weyl quantization kernel in equation (6.37) (or in (6.39) in the operator–valued case) should be adapated accordingly. In particular, the integral representation must take into account that the classical observables as well as the wave functions are only defined on a compact configuration space which in turn necessitates the use of a discrete Fourier series with respect to the respective modes instead of the continuous Fourier transform. This effectively corresponds to considering the phase space $T^*S^1 \oplus T^*S^1$ instead of $T^*\mathbb{R}^2$. We provide a derivation of the Weyl quantization formula for the phase space T^*I where I is a compact interval in appendix C. It is important to note that due to the restriction on a finite interval ambiguities occur in the definition of the momentum operator as it admits an infinite number of self–adjoint extensions (Reed and Simon 1975b). This must also be taken into account when considering the direct sum of two T^*I (we will be more precise in the next paragraph). We also refer to the work by Jorgenson, Pedersen, and Tian (2013) in this respect. In order to recover, the correct product formula for operators and hence a star product on the space of symbol functions, it is advisible to follow the detailed proof for the standard Weyl product formula by Folland (1989). We refrain here from performing this computation, and refer to the work by Stottmeister and Thiemann (2016b) in which such a restricted Weyl quantization in application to LQC has been discussed.

As anticipated above, it is necessary to clarify some domain issues regarding the quantization

procedure. In particular, we need to check whether a quantization of the homogeneous (sub) phase space associated with the variables (w, u'), namely the cotangent bundle T^*I where I is the union of the two intervals defined by $c_\pm$, is feasible. Therefore, let more generally be $I = I_1 \cup \cdots \cup I_n$ a union of disjoint intervals I_k, $k = 1, \ldots, n$. Note that the Hilbert space $L^2(I, \mathrm{d}w)$ of square integrable functions ψ over I is specified uniquely by the restrictions $\psi_k = \psi_{|I_k}$ which shows that $L^2(I, \mathrm{d}w) = \bigoplus_k L^2(I_k, \mathrm{d}w)$. Adapting the considerations to our model, each I_k is a compact and closed interval of the form $[a, b]$ with $a, b \in \mathbb{R}$. When it comes to quantization, this entails a plethora of problems because we need to impose, as mentioned above, restrictive conditions on the admissible domains of operators in order for them to be self–adjoint.

Alternatively, one can also define a new set of variables such that the new configuration variable x can take values in all of $\mathbb{R}$, and which arises from w by a suitable map. Let us consider for example

$$w = f(x) = a + \left(1 + 2\,\frac{\arctan(x)}{\pi}\right)\frac{b-a}{2}, \tag{9.106}$$

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

$$y := u'\,\frac{\partial f}{\partial x}, \quad \text{i.e.,} \quad u' = y\left(\frac{\partial f}{\partial x}\right)^{-1}, \tag{9.107}$$

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

Note however that this procedure of performing a(nother) coordinate transformation may lead to a completely different quantum theory, despite of the transformation being canonical. If one prefers to consider the quantum theory in the original positive mass squared variables (w, u', b, q') one should concentrate on defining a suitable ε–scaled Weyl calculus as refered to above. However, since the transformations are canonical in nature, one expects that the first adiabatic order of the star product and hence of the SAPT scheme does not change, as this order solely involves the Poisson bracket relations (which do not change in this case).

9.4. Identification of Slow and Fast Sectors

SAPT relies on the identification of two distinct subsystems within the model. This distinction becomes manifest by means of an adiabatic perturbation parameter ε. In the standard Born–Oppenheimer theory for molecules, the adiabatic perturbation parameter arises as the mass ratio of the light electron mass m_{e} and the heavy nuclei mass m_{n} such that $\varepsilon^2 := \frac{m_{\mathrm{e}}}{m_{\mathrm{n}}} \ll 1$. We have already

argued at the beginning of chapter 6 that such a small mass ratio together with the equipartition theorem for a standard mechanical system implies that the electrons are statistically fast compared to the heavy nucleus. In fact, together with the hypothesis of ergodicity this implies that the time average of the nuclei velocity is much smaller than the averaged electron velocity. Expressed in terms of the nuclei momentum P and the electron momentum y, this gives $\varepsilon^2\langle P^2\rangle \approx \langle y^2\rangle$. This motivates to define a rescaled nucleus momentum $p := \varepsilon P$ which gives then rise to the perturbative space adiabatic scheme. This section discusses the identificaton of slow and fast sectors in the models given before based and partially taken from (Schander and Thiemann 2019a).

This idea that one subsystem behaves much slower than another one applies to the oscillator model from section 6.8 which consists of a light harmonic oscillator coupled to a heavy anharmonic oscillator. Their respective masses m and M serve to define the small perturbation parameter $\varepsilon^2 := \frac{m}{M} \ll 1$. The system is unconstrained and the physical intuition that the heavy anharmonic oscillator moves slowly in comparison to the light harmonic oscillator follows from the equipartition theorem. In thermodynamical equilibrium at non–vanishing temperature and assuming that the system is ergodic, the phase space average, and therefore the statistical time average, of the kinetic energies are approximately equal. Then, the same reasoning as for the molecular example from above applies and one can show that the average velocity of the heavy oscillator $\dot{q}$ is much smaller than the average velocity $\dot{x}$ of the light oscillator. As explained in section 6.8.1, this statement holds true irrespective of the frequencies of the two oscillators.

The situation becomes however different for the constrained purely homogeneous and isotropic cosmological model with scalar matter content in chapter 7. First, this model does not have two mass parameters in the strict sense that could be compared one to another. However, the gravitational coupling constant $\kappa = 8\pi G$ and the matter coupling constant λ of the scalar field provide a dimensionless fraction which gives rise to a very small parameter, too, namely $\varepsilon^2 := \frac{\kappa}{\lambda}$. We note that the parameter λ is to be distinguished from the Compton wave length $1/m$ associated with the Klein–Gordon scalar field mass (where we recall that $\hbar = 1 = c$ for convenience). In the space adiabatic treatment, we assume that $\varepsilon^2 \ll 1$ which is certainly satisfied if λ is of the same magnitude as the standard length scale of the standard model, i.e., $\lambda \approx m^{-2}$. With this, we can apply the space adiabatic formalism but one might question the relevance of its use since the Hamiltonian is a constraint. The equipartition theorem is not applicable anymore and so the usual naming of slow and fast sector is lost. As we have argued in section 7.2.1, it is however possible to identify regions in the slow phase space for which one can associate the geometry with the slow sector and the matter field with the fast sector. This is possible because the Hamilton constraint is required to vanish. Most importantly, the Hamilton constraint (7.3) allows for a thorough application of SAPT. Indeed, the scheme would not be applicable if the constraint C contained inverse powers of the small parameter ε. Since C equals zero one can however always rescale C by appropriate factors of ε in order to make any inverse powers of ε disappear.

For the third model with inhomogeneous scalar field degrees of freedom and a dust scalar field the situation is different. We have a physical Hamiltonian instead of a constraint, and hence one should be very careful with rescaling the Hamiltonian by factors of ε. However, the model does not require such a rescaling. The final Hamilton function $\tilde{H}$ in equation (8.69) with the mass term $\tilde{M}$ in equation (8.70) carries only one contribution in the mass squared that is proportional to ε^2. The only inverse power in ε appears together with the cosmological constant Λ which we

assume to be so small (or even vanishing) such that it counteracts the large factor ε^{-2}.

Finally, the cosmological model with gauge–invariant perturbations in this chapter is again a constrained system. Hence, it is possible to multiply the whole Hamilton constraint by arbitrary polynomials of ε. In fact, we used this trick to arrive at the final Hamilton constraint given in equations (9.29) – (9.31). The latter is free of any anomalous terms in ε. Therefore, we also applied several rescalings of the homogenous and inhomogeneous variables that do however not impair the applicability of SAPT. The transformations of the inhomogeneous fields are canonical and hence preserve the canonical structure. The rescalings performed with respect to the homogeneous variables lead exactly to the ε–transformations of the Poisson brackets and commutator relations necessary for SAPT to work.

Eventually, let us point to an argumentation that associates the inhomogeneous degrees of freedom with a light mass while the homogeneous degrees of freedom can be identified with a heavy mass, (Schander and Thiemann 2019a). The idea is the following: Consider a three–torus (which can be assumed to be as large as the whole observable Universe) and split it into N^3 small spatial cubes with a vector $j \in \mathbb{R}^3$ pointing to their centers respectively. Integrate the inhomogeneous cosmological field over each of these small cubes and associate a new degree of freedom to each cube. This actually corresponds to a coarse graining procedure in which we replace the uncountably many field degrees of freedom by countably many "cube" degrees of freedom. The same can be achieved for the inhomogeneous conjugate momentum field. Since this is more convenenient for representing the Lagrangian and the Hamiltonian with respect to these integrated variables, one finally shifts each cube degree of freedom by the cube field at $j = 0$ (which reduces the number of degrees of freedom by one), and introduces the (new and old) mean field degree of freedom ϕ obtained by integrating over the whole torus.

Then, by evaluating the Hamiltonian with respect to the new coarse–grained variables, it turns out that one can indeed associate the homogeneous (i.e., mean field) degree of freedom with a heavy mass $M := N^3$ while the other cube degrees of freedom have mass $m = 1 \ll N^3 = M$. In a final step, one performs a unitary transformation between these cube degrees of freedom and the discrete mode degrees of freedom (which actually represent the relevant degrees of freedom for the inhomogeneous models considered here). Eventually, the homogeneous mode acquires a heavy mass while the modes associated with the inhomogeneities have a small mass. This is a proof of principle and we again refer to (Schander and Thiemann 2019a) for a more detailed account of this argument. We point however out that for unconstrained systems for which the equipartition theorem does not apply, this argument does not help to single out a "slow" subsystem. It allows however to identify certain regions in phase space (cf. the argument in section 7.2.1) in which the homogeneous mode factually behaves like a slow degree of freedom compared to the remaining inhomogeneous modes.

Part IV.

Summary and Outlook

10. Summary

In this thesis, we have examined the question of backreaction in cosmology with a focus on the backreaction problem in inhomogeneous quantum cosmology, i.e., the question of whether and to which extent the inhomogeneous cosmological quantum fields affect the global evolution of a quantum cosmological Universe. This is the first important step towards a thorough incorporation of the entire interactions between the system's constituents in non–perturbative quantum gravity plus matter. We advocate to employ the formalism of SAPT which originally goes back to Panati, Spohn, and Teufel (2003), and which allows us to rigorously study the outstanding question of backreaction in inhomogeneous quantum cosmology with a straightforward perturbative mechanism.

Our first important accomplishment is to have shown that the SAPT scheme is indeed applicable to constrained and inhomogeneous quantum cosmological models. Thereby, the constraint itself justifies the use of the adiabatic perturbation theory. We have named the conditions under which SAPT is implementable for inifinite–dimensional quantum field theories. In particular, in a first step the Hilbert–Schmidt condition needs to be met. Since the usual formulation of any cosmological QFT leads to its failure, we have specified a strategy for how to overcome this obstacle. We were subsequently able to apply SAPT to two relevant inhomogeneous cosmological models, in particular to a perturbative scalar field model with deparametrizing dust, and to the standard paradigm of gauge–invariant quantum cosmological perturbations. We emphasize that in the latter case, the usual Born–Oppenheimer scheme would not be applicable, and hence SAPT represents a substantial advancement in the application to cosmological perturbation theory. The resulting effective quantum Hamilton operator, respectively constraint, have a significantly simpler structure than their original counterparts while still taking the interactions between the homogeneous and the inhomogeneous degrees of freedom seriously into account. Solutions of these operators will lead to approximate solutions of the *full* quantum gravitational–matter problem, up to (here) errors of third order in the adiabatic perturbation parameter. Most importantly, the scheme can be carried out up to any desired perturbative order, leaving us with a powerful mechanism for approaching solutions to full quantum cosmology coupled to quantum matter.

Our findings have also entailed several new questions and research directions. We shortly point out that the scheme includes indefinite mass squared functions for the quantum fields which, if not dealt with, lead to tachyonic instabilites. We pointed to several strategies for how to circumvent these issues and applied some of them subsequently. In particular, we performed canonical transformations, respectively embeddings, of the homogeneous cosmological variables to make these mass squared functions manifestly positive. We emphasize that such instabilities already occur in standard cosmological perturbation theory, and are by no means caused by the SAPT scheme itself. We underline that a fundamental solution to this problem could be most

easily provided by inspecting the very transformations that led to these mass functions in the first place. We stress that the SAPT scheme is nevertheless applicable to quantum cosmological perturbation theory, and we were able to derive effective Hamiltonians for the above mentioned physical systems which unambigiously take the effects of backreaction into account.

In this respect, let us briefly point to one particularly interesting and astonishing outcome of the theory: Therefore, note that all effective Hamiltonians obtained with the SAPT formalism in this thesis admit non–vanishing backreaction terms due to the vacuum of the "fast" subsystem. Indeed, if we consider the backreaction induced by the fast vacuum (by setting $\nu \equiv 0$), certain contributions to the second order effective Hamiltonian for the "slow" subsystem do not vanish. In particular, the resulting Hamiltonian contains, in addition to the zeroth order "free" theory of the slow degrees of freedom, potential and even kinetic contributions. This dependence on the adiabatically "slow" degrees of freedom is actually reminiscent of the Casimir effect from quantum electrodynamics which rests on the idea that the Hamiltonian with the boundary conditions of some material interfaces is different from the free Hamiltonian, and its dependence on the position of the boundary generates a net force. In this sense, the effective Hamiltonians obtained by the SAPT scheme lead to a Casimir–like effect induced by the vacuum state of the fast subsystem exercised on the slow subsystem.

Before we will detail the possible avenues entailed by our work in the next chapter, we provide a more detailed recapitulation of our findings in the following sections.

We started with an overview of the developments in physics during the 20th century that led to the construction of the current physical standard model including general relativity and the Standard Model of particle physics. Together with high precision cosmological measurement data, this model suggests that the Universe has been expanding during its entire history and was consequently a very hot and dense place at its earliest stages. A theory of the very early Universe should hence employ the methods of QFT on CST or quantum gravity. Both approaches represent active fields of research but as it currently stands, there neither exists a fully developped theory of quantum gravity nor do we know a fully established framework for describing (interacting) QFT on CST. Nevertheless, in order to make progress in the study of the very early Universe, possible ideas are to employ suitable approximation schemes and exploit known symmetries of the system. This leads to the theory of linear perturbative quantum cosmology which should be relevant when the inhomogeneities of the system are small compared to the purely homogeneous contributions to the system. The usual proceeding of these approaches consists in propagating the inhomogeneous quantum fields on a formerly fixed effective quantum background. Then, backreactions of the inhomogeneous quantum fields on the global evolution of the dynamical (quantum) background are neglected. Hence, these procedures dismiss important effects of the interactions within the system.

Of course, the problem of neglecting backreaction plays also a role in purely classical considerations of the late time classical Universe, and we reviewed the current methods to examining such classical backreaction. There are several proposals for how to approach this question (e.g., non–perturbative and perturbative models, different matter configurations etc.) but no conclusive answer has been given so far due to the mathematical and physical complexity of the problem. One important issue concerns the choice of the reference volume in the procedure of averaging which is evidently a physical and not a gauge choice.

The same question concerning backreaction effects arises in semiclassical frameworks in which one describes the inhomogeneous cosmological perturbations using QFT and the geometry by means of classical general relativity. We reviewed the approaches of semiclassical gravity and stochastic (semiclassical) gravity that address the backreaction problem within QFT on CST. In both cases, one first needs to find admissible quantum states for evaluating the expectation value of the matter stress–energy tensor in order to find, in a second step, solutions to the modified classical Einstein equations which include this expectation value (and possibly further "stochastic" contributions) as additional sources. Due to the generic difficulties of identifying suitable states that lead to a well–defined expectation value of the stress–energy tensor on a generically curved space time (e.g., due to UV–divergences, identifying a suitable regularization and renormalization procedure, ambiguities of quantum states in generically curved space times), this endeavor is not a trivial one, and only realized for certain (rather simplistic) matter contents. Also the second stage of finding solutions to the modified Einstein equations turns out to be involved as one has to deal with stability problems, in particular for non–trivial matter configurations. Furthermore when considered from a conceptual point of view, the semiclassical approach leaves us with the question of whether one should couple purely quantum mechanical fields to a classical gravitational field. Although, it seems to be a physically reasonable approach in situations where quantum effects of gravity are negligible while matter shows quantum behavior, the mathematical frameworks are per se incompatible.

To approach a purely quantum mechanical discussion of the problem, we reviewed the known avenues to the question of backreaction within several approaches to quantum gravity and quantum cosmology. We focused on those ideas that employ a perturbative expansion with respect to the tiny inverse Planck mass and more precisely, those approaches that use Born–Oppenheimer like methods. Besides, we discussed the relation between those perturbative approaches and the semiclassical limit to quantum gravity which are closely related but actually independent. Therefore, the question of quantum backreaction can be considered independently of the semiclassical limit, and which we have done in this thesis. While considering the semiclassical limit is a perfectly legitimate procedure, most importantly to bridge the gap between theory and observations, it is also of unconditional relevance in order to independently understand the interactions of the system's components within a pure quantum gravitational formalism. Most of these approaches additionally employ however a semiclassical limit, choosing very specific semiclassical ansatz solutions, or must remain on a formal level due to the high complexity of the theories. Moreover, they are subject to the limitations of the standard Born–Oppenheimer theory, namely the coupling must be provided by mutually commuting operators of the slow sector, and the perturbative scheme cannot be extended to higher, improved error estimates. We therefore strongly suggest to make use of the correspondingly revised scheme of SAPT.

To make this point clear, we reviewed the Born–Oppenheimer scheme, thereby focussing on its properties that prevent its application to the cosmological models that we have in mind, namely the requirement of a common spectrum of the coupling operators associated with one part of the system. As it turns out, SAPT overcomes these shortcomings by employing a phase space quantization scheme for this sector of the model. The latter also allows to define a perturbative scheme up to any desired order in the corresponding adiabatic perturbation parameter. We subsequently reviewed the basics of Weyl quantization, phase space quantum mechanics and operator–valued

pseudodifferential calculus which are the basis of SAPT. After introducing the conditions and the construction scheme of SAPT, we gave a detailed iterative account of the construction procedure and also provided a more detailed set of formulae for the scheme up to second perturbative order.

As a first exercise, we applied the space adiabatic perturbation formalism to a simple toy model consisting of a fast harmonic oscillator coupled to a slow anharmonic oscillator. The coupling is provided here by the potential energy of the two oscillators. The adiabatic perturbation parameter is defined as the mass ratio $\varepsilon^2 := \frac{m}{M}$ of the light harmonic oscillator of mass m and the heavy anharmonic oscillator of mass M with $m \ll M$. Due to the equipartition theorem, the anharmonic oscillator can be identified as the slow subsystem compared to the fast harmonic oscillator. Although the model consists of only two degrees of freedom which a priori allows for a direct application of SAPT, the Hamilton operator does not satisfy the four outlined conditions of the SAPT scheme because it is an unbounded operator with respect to the fast subsystem, and furthermore is an anbounded function with respect to the slow phase space variables. As suggested by Panati, Spohn, and Teufel (2003), we therefore defined an auxiliary Hamiltonian whose Wigner–transformed symbol function belongs to an appropriate symbol class such that SAPT can be applied to this problem. However, this Hamiltonian is physically different from the original Hamiltonian, and it is not possible to assure the convergence of the perturbative series associated with the original problem by this procedure. This is due to the fact that the latter is an unbounded operator. One must hence either employ the auxiliary (inequivalent) Hamiltonian which would guarantee the convergence of the problem, or remain with the original Hamiltonian without a manifest result regarding the convergence of the perturbative series.

The resulting effective Hamiltonian derived from the original Hamiltonian and up to second order in the adiabatic perturbations includes a standard Born–Oppenheimer zeroth order part and a non–trivial second order contribution. We solved the quantum problem for the anharmonic oscillator subject to the backreactions of the harmonic oscillator by using standard quantum mechanical perturbation theory. This is possible because the zeroth order effective Hamiltonian has a pure point spectrum. In particular, the zeroth order problem has the form of a harmonic oscillator with an off–set energy and frequency that both depend on the backreaction of the fast oscillator. The second order effective Hamiltonian includes kinetic as well as potential energy contributions and depends non–polynomially on the position variable. Using quantum mechanical perturbation theory, we computed the second order spectral shift which depends on the backreaction from the fast oscillator.

As a second, also still quantum mechanical model, we considered a homogeneous and isotropic cosmology with a cosmological constant and coupled to a real–valued massive scalar particle. The geometric sector of the theory naturally arises as the ε–scaled subsystem where the perturbative parameter ε arises as the ratio of the gravitational and the matter coupling constant. Since the system is completely constrained, the usual assignment of slow and fast sectors due to the equipartition theorem fails. Nevertheless, we can identify regions in the geometric phase space for which the standard interpretation of slow and fast variables is restored. In either case, we emphasize that SAPT applies as soon as one can determine a suitable perturbation parameter and if the Hamiltonian has a certain form. Namely, it should not carry inverse powers of ε which would impair the perturbative scheme. However, in the case of constrained systems this represents no problem as one can simply multiply the whole constraint by appropriate factors

of ε. In the given example, such an inverse factor appears only together with the cosmological constant which we assume to be so small such that it does not harm our results. Consequently, we are able to compute an effective quantum Hamilton constraint for the geometry including the backreaction from the scalar field. The resulting theory at zeroth order is an inverse oscillator which is known to have a continuous real spectrum. Unfortunately, this implies that the standard quantum mechanical perturbation theory for evaluating the second order effective Hamiltonian is not available anymore, and we leave the further examination of the spectral problem for future research.

The third model considered in this thesis finally applies SAPT to a quantum field theoretical cosmological model. More precisely, in this model the purely homogeneous geometry is coupled to an inhomogeneous Klein–Gordon field and a deparametrizing timelike dust field. Besides, it includes a cosmological constant. Technically, the space adiabatic scheme first requires us to consider the inhomogeneous QFT on a classical dynamical background. However, we show that the QFTs for different background configurations are physically inequivalent in the sense that the Hilbert–Schmidt condition is violated, i.e., the vacua for different background configurations cannot be related by a suitable (or even unitary) transformation – they live in different Hilbert spaces. This corresponds however to an (unsaid) important condition for the functioning of SAPT, more concisely the "fast" fibre Hilbert spaces of the QFT's must all be the same. We find a solution to this obstacle by employing transformations for the whole canonical system that are canonical up to second order in the cosmological perturbations, and which were previously introduced in the hybrid approach to LQC. The implementation of such transformations allows us to apply SAPT, however at the cost of introducing an effective mass squared for the quantum field that is an indefinite function of the homogeneous geometry. Hence, the theory admits a priori tachyonic instabilites at least for certain homogeneous configurations.

Fortunately, such instabilities can be circumvented by means of a transformation for the geometric sector as we show in the corresponding chapter. The application of the scheme up to second perturbative order then provided us with an effective Hamiltonian for the homogeneous sector including the backreaction of the inhomogeneous quantum Klein–Gordon field. At zeroth order, we regained the homogeneous geometric quantum operator together with an effective potential energy contribution from the Klein–Gordon quantum energy bands. This corresponds in fact to the standard Born–Oppenheimer outcome – which is little surprising since this model would have also allowed for an application of the Born–Oppenheimer scheme as the coupling is provided solely by the geometric configuration variable. However, the non–vanishing second order effective Hamiltonian goes beyond the standard Born–Oppenheimer scheme and yields a number of corrections that in part depend on all possible energy bands of the Klein–Gordon field. In particular, there are backreactions from the vacuum of the QFT. Despite the infinite sums, these contributions converge but also depend non–polynomially on both, the geometric configuration variable and its conjugate momentum which aggravate the quest for a suitable domain of the Hamilton operator and its solutions. However, it is possible to name a domain for a certain class of non–polynomial mixed operators in section 7.2.2.

The final model and centerpiece of this thesis is a standard inhomogeneous cosmology that consists, on the one hand, of the standard homogeneous and isotropic sector of geometry and a massive Klein–Gordon scalar field, and on the other hand, its associated gauge–invariant linear

perturbation fields. This system is completely constrained and we hence performed a Dirac analysis in order to obtain the relevant constraints. Together with the transformations that prevent the Hilbert–Schmidt condition from failing for the corresponding QFT, we obtained a single non–trivial Hamilton constraint that describes the physical properties of the system. Its zeroth order contribution has the standard form of the purely homogeneous cosmological Hamilton constraint while its second order consists of a pure Mukhanov–Sasaki and graviton part (the vector perturbations are naturally solved by the scheme itself). Both the scalar and the graviton perturbative fields have the form of a minimally coupled real scalar field whose effective masses squared, again, depend on the homogeneous degrees of freedom.

First leaving the problems associated with tachyonic instabilities aside, we applied SAPT to this model and obtained an effective Hamilton constraint for the homogeneous geometry and Klein–Gordon system that includes the backreaction from the Fock perturbations. At zeroth order we obtain the usual Born–Oppenheimer–like contributions that consist of the homogeneous constraint as well as a "bare" energy from the relevant Fock perturbation energy bands. The first order contribution is again vanishing. A careful analysis of the second order contribution, in particular of its ε–scaling of every term, results in a one–line formula for the contributions proportional to ε^2. At this order, any tensor backreaction vanishes and we are left with the Mukhanov–Sasaki contributions. They contain sums over the whole $k \in \mathbb{k}$ and with respect to the frequency function $\omega(k^2)^{-5} = (k^2 + M^2_{\mathrm{MS}})^{-(5/2)}$. If M^2_{MS} is positive the sum will converge. However, we saw that M^2_{MS} is an indefinite function leading to divergencies of the symbol function. Moreover, the whole effective symbol Hamilton constraint depends non–trivially on the homogeneous phase space variables which substantially complicates the quest for a domain of the constraint and possible solutions.

Therefore, we discuss several proposals for how to overcome the issues related to the indefinite masses squared and the corresponding tachyonic instabilities. The first proposal goes back to the point where the indefinite mass squared functions occured – namely when transforming the phase space of the theory in order to have well–defined QFTs. In our applications, we restricted to the simplest possible transformations and followed the paths proposed by Castelló Gomar, Martín-Benito, and Mena Marugán (2015) and Martínez and Olmedo (2016). It is hence possible that a further examination of the possible transformations yields mass functions that avoid the tachyonic instabilities right from the beginning. A second proposal is to restrict the homogeneous phase space in a suitable manner such that the masses squared become manifestly positive. This can be achieved by finding a suitable canonical transformation in the homogeneous sector that leads to a positive mass squared. Such a strategy has actually been employed for the inhomogeneous model with dust field, and we also discussed a corresponding modification of the model with gauge–invariant cosmological perturbations in the last chapter. The resulting effective Hamilton constraint for the transformed homogeneous degrees of freedom is of a similar form but also contains the backreaction from the tensor modes. This is not very surprising since such a procedure is likely to change the resulting quantum theory. In fact, it is well known that a canonical transformation on the classical level will probably yield a different quantum theory. This is not problematic per se, the experiment has to show which choice of variables is physical.

In this respect, we also point out that transformations for positive mass squared functions possibly restrict the original phase space in that the new variables are only defined on compact

subsets of the original phase space. This is the case in the given model and consequently, the Weyl quantization procedure underlying the Moyal product and hence the SAPT scheme must be carefully revised. Again, the resulting effective Hamilton constraint depends on $\omega_{\mathrm{MS}}(k^2)^{-5}$, and also on $\omega_{\mathrm{T}}(k^2)^{-5}$, which are being summed over all possible modes. Since the mass squared functions are both positive definite in terms of the new variables no tachyonic instabilities occur and the sums converge. However, the effective Hamilton constraint still depends in a non–trivial and non–polynomial way on the homogeneous degrees of freedom which makes the search for a domain of definition and possible solutions of the quantized constraint more difficult. We leave this for future research, and point again to a proposal for such a domain.

We also pointed to the possibility of restricting the admissible perturbative modes for every point (q, p) in the slow phase space by hand such that the frequency functions do not admit imaginary values. This leads however to complications for the SAPT scheme which by itself relies on "connecting" the different fibre Fock spaces on the homogeneous phase space. For example, the Moyal symbol $\boldsymbol{u}$ that links subspaces of the Fock spaces at different points (q, p) would not be unitary anymore. A fourth possibility is to modify the Weyl quantization procedure by restricting the integrals entering the Weyl integral representation to the regions in phase space for which the mass squared functions are manifestly positive. To soften this adhoc cut–off, it is possible to multiply all symbol functions by a suitable smoothed characteristic function which however modifies the quantization procedure, and hence the physical results, itself.

Finally, we emphasized that the space adiabatic scheme applies in principle to every model that admits a suitable perturbative parameter arising as the ratio of the masses or coupling constants of two respective subsystems. In case of a true, physical Hamiltonian, the system should furthermore avoid inverse powers of the perturbative parameter as this would impair the perturbation theory. For a constrained system whose Hamiltonian is forced to vanish, it is possible to multiply the whole constraint by appropriate factors of the perturbative parameter in such cases. However, the standard reasoning that the subsystem with the heavy mass evolves with a smaller velocity than the light subsystem does not transfer to the constrained case (and is also not necessary). In fact, this reasoning goes back to the equipartition theorem and the ergodic hypothesis which are only applicable to unconstrained systems. Nevertheless, the purely homogeneous cosmological model still allows to identify the geometry with the slow sector and the scalar field with the fast sector for certain regions in phase space. In fact, as soon as the Hamilton constraint is satisfied classically, the constraint equation serves for identifying these regions.

A similar argumentation is also possible for constrained *inhomogeneous* systems, see section 9.4 and (Schander and Thiemann 2019a) in which case we would like to identify the homogeneous mode with the slow sector. Such an argument can be made manifest by performing a coarse graining procedure in which one subdivides the whole space time manifold (here the three–torus) into a large number $N^3 \in \mathbb{N}^3$ of equally sized spatial volumes. These inhomogeneous "cube" degrees of freedom can be unitarily related to the discrete modes of the inhomogeneous field (i.e., the relevant inhomogeneous degrees of freedom in the inhomogeneous models encountered here). Then, the purely homogeneous (mean field) degree of freedom automatically acquires a heavy mass $M := N^3$ which is much larger than the masses $m := 1$ associated with the inhomogeneous modes. This can be seen by evaluating the corresponding Hamilton constraint. Then, the above argument for identifying slow and fast sectors in certain phase space regions used for the

purely homogeneous case, applies to these inhomogeneous models as well.

11. Outlook

In this final section, we would like to provide the reader with some of the most interesting open questions entailed by our findings and propose several new research directions associated with these questions (and which are also partly already under investigation).

One possible extension of our application of SAPT to the four given models is of course to pursue the perturbative scheme up to higher perturbative orders. We have worked out the scheme up to the second order but the construction of higher order estimates is possible and straightforward. We have laid the basis for such an enterprise in section 6.6 where we have detailed the iterative construction of the perturbative scheme at every possible order. In the concrete applications, we have however restricted to second order considerations since the computations become quickly heavy. Nevertheless, such extensions would be particularly interesting in order to check whether the scheme converges in an obvious way, for example one might think that the effective Hamiltonians encountered in the inhomogeneous models will be proportional to $\omega(k^2)^{-n}$ for a suitable $n \in \mathbb{N}$ and hence sum up to a convergent contribution.

As pointed out earlier, the effective Hamiltonians obtained in chapters 8 and 9 include mass functions of the perturbative quantum fields whose squares are indefinite functions of the homogeneous variables. This might lead to tachyonic instabilities. While we have implemented solutions to this issue by performing transformations within the homogeneous sector only, it seems natural to first scrutinize the very transformations introduced in sections 8.1 and 9.1 that led to such mass functions. We emphasize once more that such indefinite mass functions already occur in the standard gauge–invariant cosmological perturbation theory, and are not exlusively due to the application of SAPT. We have pointed out that there is a tremendous freedom in the choice of such transformations, and which should be investigated further. Unfortunately, this could not be done within the time limitations of this thesis. One immediate idea leading to a more generic set of transformations is to allow these to depend on the Laplace–Beltrami operator.

Other proposals for circumventing the tachyonic instabilities would be to restrict the homogeneous phase space to regions in which the mass squared functions are manifestly positive. For such an enterprise, one needs to review the Weyl quantization scheme for these homogeneous variables and take care of possible domain issues. We underline that a thorough examination of the field transformations as proposed before would make this investigation obsolete. Due to these indefinite mass squared functions, the final spectral analysis of the effective Hamiltonians obtained so far has not been carried out yet. Once this technical problem is fixed, the scheme will allow us to make considerable progress in the yet unanswered question of quantum backreaction, and consequently lead to a more profound understanding of the interactions between gravity and matter in the very early Universe. Moreover, our formalism is not only a promising tool in the quest of purely quantum field theoretical solutions for these earliest moments but is also ideally suited to bridge the gap between theory and experiment. In fact, we have seen that the adiabatic

limit (invoked here) and the semiclassical limit go hand in hand, which will ultimately allow us to confront our theoretical results with observations.

Fortunately, there are a variety of observational findings, such as the recent acceleration of our Universe, the dark matter problem, the H_0– and possibly the S_8–tension and many more, that reveal a discrepancy between our current cosmological models and reality. On the other hand, the ever increasing abundance of cosmological data of ever increasing precision allows us to poinpoint the shortcomings of the concordance model, and to scrutinize the possible modifications of the inflationary ΛCDM model. In this respect, we take a novel but at the same time conservative position and pursue an approach that is long overdue: We advocate to include the yet missing fundamental backreaction in theories of quantum gravity plus matter, and to first fully understand the underlying interactions before introducing very novel ideas into the game. This will finally enable us to tackle the question of finding possible fingerprints of quantum gravity in cosmological data. We hence venture to ask the question whether the inclusion of backreaction might possibly be sufficient to account for the outstanding problems of modern cosmology, or if they will, at least, provide partial answers.

One excellent avenue in this direction is to use our quantum cosmological models with perturbations, including backreaction effects, to generate primordial and eventually angular CMB power spectra, which can then be compared to the recent measurements by the Planck collaboration, (Aghanim et al. 2020a), or to the even more precise measurements of future CMB missions. Thereby, we might introduce a semiclassical approximation scheme while still accounting for the backreaction between inhomogeneous and homogeneous degrees of freedom. This could for example be done by introducing suitable semiclassical states with respect to the homogeneous sector. This will provide us with a standard cosmological QFT on CST in which the cosmological perturbations propagate on the homogeneous background. One other possibility to regain the semiclassical limit within SAPT was proposed by Teufel (2003): Using Egorov's theorem, we know that the evolution of the quantum mechanical perturbations with respect to the homogeneous degrees of freedom can be obtained by transporting the perturbations along the classical flow generated by the original Hamiltonian constraint. In this approach, the evolution of the perturbations will simply follow the classical trajectory provided by the energy eigenvalue of the zeroth order Hamiltonian symbol problem (up to errors of second order in ε). Any higher order contribution can be obtained by expanding the Heisenberg evolution equation in a phase space quantization scheme. This scheme as proposed by Teufel (2003) applies to unconstrained systems but by using the quantum constraint equation instead of the Heisenberg equation, one should obtain similar results for the constrained case. After following their evolution until the time of photon decoupling, intercepting the mode amplitudes will allow us to compute the power spectrum of scalar perturbations.

In this respect, we also point to the existing anomalies observed in the CMB such as the power suppresion at large angular scales, the dipolar asymmetry, a preference for odd–parity correlations and the tension associated with the lensing amplitude (Aghanim et al. 2020a). In fact, it has recently been shown that certain (quantum) modifications of the standard model at earliest times can be responsible for these anomalies (Agullo, Kranas, and Sreenath 2021), and which are particularly mediated by non–Gaussianities of the perturbations. In fact, we also expect that the scalar field in our models will admit self–interactions when taking higher order perturbations in

the inhomogeneities into account. Such self–interactions could significantly contribute to cosmological non–Gaussianities, and which would be naturally produced by the SAPT formalism. We point to already existing higher order schemes in the existing literature (Brunetti, Fredenhagen, Hack, et al. 2016; Dittrich and Tambornino 2007a,b), and which could be implemented in our SAPT scheme.

We also mention that the inclusion of backreaction with the SAPT scheme could provide a natural answer to the problem of cosmological singularities in the very early Universe. Indeed, the backreaction effects may, even at the purely homogeneous and isotropic level, lead to modified quantum constraint equations that naturally solve the singularity problem. The quest for solutions of the effective Hamiltonians derived within the scope of this thesis represents hence a project of compelling importance.

12. French Summary – Compte–Rendu Français

Résumé

Cette thèse aborde le problème des réactions inverses en cosmologie. Plus précisément, nous cherchons à donner une réponse à la question de la signification et de la forme des effets excercés par les inhomogénéités cosmologiques sur l'évolution globale de l'Univers et cela dans un cadre purement quantique. Nous nous concentrerons donc, mais sans nous y limiter, sur les réactions inverses quantiques adaptées pour décrire les premières phases de l'Univers. Notre approche se sert d'un formalisme perturbatif et constructif nommé théorie des perturbations spatio–adiabatiques et qui s'inspire de l'approximation de Born–Oppenheimer bien connue de l'analyse spectrale des systèmes moléculaires. Cette théorie développe l'approche de Born–Oppenheimer de plusieurs façons.

L'idée sous–jacente de cette approche consiste à séparer le système en une partie adiabatiquement lente et en une partie rapide, similaire à la séparation des sous–systèmes nucléaires et électroniques dans un molécule. Une telle distinction est raisonnable si un paramètre perturbatif correspondant peut être identifié. Dans le cas des systèmes moléculaires, un tel paramètre provient de la fraction des masses des électrons légers et des noyaux lourds. En cosmologie par contre, nous identifions le rapport des constantes de couplage de la gravitation et de la matière comme un paramètre perturbatif susceptible. Dans une première étape, nous appliquons ce formalisme spatio–adiabatique à un modèle d'oscillateurs simples ainsi qu'à un modèle cosmologique réduit de symétries comprenant un champ scalaire couplé à la géométrie d'espace–temps. Nous réussissons à dériver des opérateurs hamiltonien effectifs dans les deux cas qui comprennent les réactions inverses du système rapide excercés au système lent. Nous nous limitons à des calculs au second ordre dans les perturbations adiabatiques.

Par la suite, nous appliquons la théorie des perturbations spatio–adiabatiques à des modèles de cosmologie inhomogène et calculons les effets des réactions inverses des champs cosmologiques quantiques et inhomogènes sur les degrés de liberté quantiques globaux (par exemple sur le taux d'expansion de l'Univers). Pour cela, il est nécessaire d'étendre le schéma de manière adéquate pour permettre son application aux théories des champs de dimension infinie. Plus précisément, la violation de la condition de Hilbert–Schmidt dans le contexte des théories quantiques des champs empêche l'application directe du schéma. Il s'avère qu'une transformation des variables (au niveau classique) qui est canonique jusqu'au second ordre dans les perturbations cosmologiques offre une solution à ce dilemme. Ces transformations nous permettent de calculer un opérateur hamiltonien effectif pour une théorie cosmologique des champs quantiques, préalablement déparamétrisée par un champ de poussière, ainsi que l'identification d'une contrainte

hamiltonienne effective pour un système comprenant des perturbations cosmologiques invariantes de jauge. Les deux objets agissent sur les degrés de liberté globaux et incluent les effets des réactions inverses des inhomogénéités jusqu'au second ordre spatio–adiabatique.

Nous concluons par souligner qu'il est a priori inadmissible de négliger les effets de réaction inverse en cosmologie selon nos résultats. Cependant, en raison des difficultés générales associées à la recherche de solutions pour les systèmes gravitationnels couplés à la matière, l'évaluation concrète des opérateurs trouvés ici reste le sujet de recherches futures. Un obstacle est l'apparition de carrés de masse indéfinis associés aux champs perturbatifs qui sont le résultat des transformations mentionnées ci–dessus. Une autre complication dans la quantification finale et la recherche de solutions appropriées provient de la dépendance non–polynomiale des degrés de liberté globaux. Nous discutons ces obstacles en détail et indiquons des solutions possibles.

I. Introduction

I.1. Réactions Inverses et Modèle Standard de Physique

Ce premier chapitre entend présenter succinctement les principes du "modèle standard" de la physique contemporaine qui représente également la base pour ce projet de thèse. Il s'agit d'un voyage chronologique à travers la physique des XXe et XXIe siècles.

Notre expédition commence par la découverte fondamentale d'Einstein que l'espace–temps représente une entité dynamique symbolisée par le champ gravitationnel et dont la dynamique est directement liée au contenu matériel et à l'énergie du système. Cette relation se manifeste dans les équations covariantes d'Einstein qui forment la base de la relativité générale. Malheureusement ces équations différentielles d'ordre deux et non–linéaires ne nous offrent pas de solutions en général, mais leur application à l'Univers entier peut profiter des symétries inhérèntes au système. Plus précisément, les observations cosmologiques indiquent que l'Univers était spatialement homogène et isotrope (dans un sense statistique) à des petites perturbations près pendant ses phases anciennes, et il l'est encore aujourd'hui sur des échelles supérieures à environ 100 Mpc. Supposons pour un instant que l'Univers était purement homogène et isotrope, cela signifie une simplification énorme pour les dégrés de liberté admissibles et les équations dynamiques de la théorie. Il en résulte la métrique FLRW ainsi que les équations de Friedmann–Lemaître qui déterminent l'évolution de l'Univers une fois que le contenu de matière est connu et bien sûr sous l'hypothèse d'homogénéité et d'isotropie.

Cette théorie nous conduit au modèle standard de la cosmologie contemporaine et sa simplicité a sûrement contribué à stimuler l'intérêt en cosmologie et à la collecte de données cosmologiques. La quantité des données de mesure recueillies entre–temps est remarquable et, avec les fondements théoriques, elle nous permet de retracer l'histoire de l'Univers à plus de 13 milliards d'années. Dans ce cadre, les inhomogénéités de l'Univers sont décrites par de petits champs perturbatifs. Dans les époques récentes et donc classiques, ces champs inhomogènes sont décrits

comme des champs classiques qui n'impactent pas le fond homogène et isotrope. Pendant des époques plus anciennes, on suppose qu'au moins les champs de matière doivent être considérés dans un formalisme de mécanique quantique, on se sert plus précisément d'une théorie quantique des champs sur un espace–temps courbe. Durant les premières phases de l'Univers, nous partons du principe que tous les degrés de liberté doivent être considérés dans un formalisme quantique, les champs inhomogènes ainsi que les dégrés de libertés globaux. De la même manière que dans le cas purement classique, ces théories quantiques ou semi–classiques propagent les champs inhomogènes sur un fond classique ou effectif semi–classique sans tenir compte des réactions inverses de ces inhomogénéités sur le fond.

Cela est dû, bien sûr, à la complexité des théories concernées. Danc ce chapitre, nous identifions les difficultés diverses rencontrées pour comprendre et décrire de manière adéquate les interactions et réactions inverses des différentes parties d'un système quantique ou semi–classique. Nous faisons référence au problème (non–résolu) de formuler une théorie des interactions quantiques au niveau mathématique, le théorème de Haag, la non–renormalisabilité de la gravité quantique perturbative, les ambiguïtés de définir un vide en théorie quantique des champs en espace–temps courbe et la possibilité de rencontrer des représentations inéquivalentes en théorie quantique des champs.

Nous proposons donc de recourir à un schéma d'approximation qui permet de trouver des équations effectives ou des solutions physiques au moins approximatives. En particulier, nous abordons l'idée de l'approche de Born–Oppenheimer bien connue de la physique des molécules et qui emploie le rapport de la petite masse des électrons et la grande masse des noyaux comme un paramètre perturbatif. Cependant, l'approche considère les deux sous–système sur un niveau quantique. Nous soulignons que cette idée s'applique également aux systèmes contraints en gravitation mais qu'une extension du formalisme est nécessaire. En effet, une telle extension a déjà été élaborée pour des systèmes de mécanique quantique, à savoir la théorie des perturbations spatio–adiabatique. Le but de cette thèse est d'appliquer ce formalisme aux modèles cosmologiques et de l'étendre pour une application en cosmologie inhomogène.

II. Contexte de Recherche

II.2. Relativité Générale et Cosmologie Standard

Ce chapitre entend donner un court résumé des bases de la relativité générale et de la cosmologie standard, plus précisément du modèle ΛCDM avec de l'inflation. Il s'agit, dans une première étape, d'énoncer les notions élémentaires de la relativité générale mais aussi d'introduire le formalisme ADM et l'analyse des contraintes (selon Dirac) qui sont rarement présentés dans les introductions à la relativité générale. Dans une deuxième étape, le chapitre présente les bases théoriques de la cosmologie contemporaine qui s'appuient surtout sur la relativité générale, la théorie quantique des champs en espace courbe et des principes de symétrie. Bien que la cos-

mologie physique est incontestablement un des grands succès scientifiques du dernier siècle, nous insisteront finalement sur les incomplétudes et les inconsistences du modèle.

Néanmoins, on commencera par s'adresser aux grandes réussites de la cosmologie physique. L'observation du fond diffus cosmologique, l'analyse du spectre des galaxies et la détection des ondes gravitationnelles des trous noirs binaires sur Terre ne représentent que quelques exemples des acquis scientifiques exceptionnelles dans le domaine de la cosmologie. La relativité générale donne un cadre théorique pour tenir compte de ces phénomènes divers. Elle est basée sur l'idée que l'espace–temps est déformé par le contenu de matière et son énergie. Les équations de champ d'Einstein exhibent ce lien entre les composantes matérielles du système et du champ gravitationnel qui représente sa géométrie. Ces équations sont soumises au principe de covariance généralisé qui constitue le principe fondamental de la théorie. Pour autant, il est souvent considéré comme désirable de suivre un formalisme hamiltonien qui permettra d'accomplir une quantification canonique. Le formalisme ADM réalise une telle énonciation hamiltonienne de la gravitation. Pour en déduire les solutions physiques de la théorie, il faut suivre une analyse des contraintes. Cette analyse de même qu'une quête des solutions aux équations d'Einstein (qui sont des équations différentielles d'ordre deux et non–linéaires) s'avèrent compliquées et ne sont pas accessibles dans des situations générales.

Pour établir une théorie physique qui est néanmoins capable de décrire les phénomènes cosmologiques mentionnés ci–dessus, on suppose l'Univers spatialement homogène et isotrope et constitué d'un fluide parfait. À partir des ces symétries, on peut facilement établir une métrique qui est entièrement déterminée par un facteur de courbure fixé k et le facteur d'échelle a – c'est la métrique de Friedmann–Lemaître–Robertson–Walker. Les équations d'Einstein se réduisent aux équations de Friedmann–Lemaître qui guident l'évolution de l'Univers, concurremment avec l'équation de continuité. Tenant compte des observations et des propriétés connues de la matière, cette théorie trace l'histoire d'un Univers en expansion permanent qui débute dans un état de densité d'énergie infinie – le "Big Bang". Pour résoudre les problèmes inhérents de l'horizon et de la platitude, le modèle ressort à un champ scalaire réel – dit inflationnaire – présent aux premiers instants de l'Univers. D'ailleurs, la théorie est enrichie des perturbations cosmologiques linéaires qui tiennent compte des inhomogénéités présentes, par exemple, dans le CMB. Il est supposé que ces perturbations n'influencent pas l'évolution du fond homogène et isotrope.

Malgré son succès, ce modèle simpliste de l'Univers présente des défauts essentiels. Du côté observationnel, on est confronté au fait que l'Univers est composé de 94% d'énergie et de matière noire dont la nature est toujours inconnue. D'ailleurs, diverses mesures de la constante de Hubble arrivent à des résultats incompatibles. Il semble donc urgent de réviser ce modèle. Notre approche (conservatrice) à ce sujet est d'inclure des réactions inverses des inhomogénéités qui ont été négligées dans une première étape.

II.3. Réactions Inverses Classiques

Ce chapitre entend exposer une introduction aux approches purement classiques des réactions inverses en cosmologie. Plus précisément, il s'agit d'évaluer des effects des inhomogénéités cosmologiques sur l'évolution globale de l'Univers et cela dans un formalisme classique. Les méthodes présentées sont qualifiées donc pour décrire des réactions inverses dans l'Univers "récent" c'est–à–dire après le découplage de matière et de radiation. Ce domaine de réactions inverses classiques comprend plusieurs méthodes distinctes et la théorie s'applique à des modèles de contenu de matière variés. Aussi diverses que soient les techniques, les résultats le sont aussi. En effet, il n'y pas d'accord sur l'intensité et sur la forme de ces réactions. Pour structurer notre résumé, nous avons distingué d'un côté des méthodes analytiques non–perturbatives et perturbatives et de l'autre des simulations numériques.

Nous commençons par noter que les équations de Friedmann utilisées en cosmologie standard ne sont correctement valides que dans un système qui est *exactement* homogène et isotrope en ces dimensions spatiales. Étant donné que notre Univers a toujours compris des inhomogénéités, par exemple apparentes dans le fond diffus cosmologique et dans la distribution de matière présente, il faut réviser les équations dynamiques pour l'Univers à des échelles globales. En partant des équations d'Einstein locales dont la validité a été montrée à haute précision, il faut trouver une méthode pour en obtenir une "moyenne" judicieuse. Nous présentons les deux méthodes les plus connues: le schéma des moyennes scalaires de Buchert et la méthode covariante de Zalaletdinov dites "gravité macroscopique". Ces deux techniques s'appliquent aux modèles non–perturbatifs ainsi qu'aux modèles perturbatifs, mais dans tous les cas elles sont soumises à des ambiguités importantes pour les résultats physiques. Le choix des coordonnées et donc le choix du volume moyenné ainsi que le modèle du contenu de matière y jouent un rôle important. Nous présentons plusieurs applications de ces méthodes à des modèles divers et soulignons leurs résultats différents. En outre, on fait référence à des études en cosmologie inhomogène qui ne consistent pas à calculer des moyennes mais qui cherchent à suivre l'évolution exacte de modèles simplistes de l'Univers. À ce sujet, on mentionne, entre autres, les modèles de "fromage suisse", de "Timescape Cosmology" et la formule de Lindquist–Wheeler d'un univers sur réseau.

Nous continuons avec les approches perturbatives, applicables dans des situations avec des inhomogénéités petites qui s'utilisent donc surtout aux phases anciennes de l'Univers. Elles permettent d'analyser le problème des réactions inverses en espace Fourier des champs de perturbations cosmologiques et donc de recourir à des spectres de puissance primordiaux pour falsifier les résultats. Étant donné l'exiguïté des perturbations, les études effectuées indiquent que les effets inverses sont plutôt négligeables. Néanmoins, plusieurs questions restent pendantes dues aux coupages artificiels de modes infrarouges et ultraviolets. Au dernier paragraphe, nous abordons aussi les réactions inverses dues aux perturbations cosmologiques dans des modèles inflationnaires de l'Univers primordial. Il s'avère que ces réactions impactent la loi de Hubble–Lemaître sur des échelles locales.

Finalement, nous attirons l'attention de la lectrice/ du lecteur sur des simulations numériques qui ont seulement été effectuées récemment. Elles retracent l'évolution des perturbations pendant les phases classiques de l'Univers pour en déduire les effets de réactions inverses. En fonction du modèle de matière sous–jacent, ces études trouvent des effets négligeables ou des

corrections de 15% au taux d'expansion de l'Univers.

II.4. Théorie Quantique des Champs en Espace–Temps Courbe

La théorie quantique des champs est un des piliers de fondation du modèle standard de la physique contemporaine. Dans une première étape, ce chapitre entend récapituler les bases de la théorie quantique des champs en espace–temps courbe qui constitue aussi le fondement de cette thèse. À ce sujet, nous commençons par aborder une approche covariante dans un formalisme de théorie quantique des champs *algébrique* qui est particulièrement susceptible de tenir compte des caractéristiques d'un espace–temps courbe. D'ailleurs, nous retraçons les idées de l'approche hamiltonienne à la théorie quantique des champs ce qui est bénéfique pour une quantification canonique par la suite. La deuxième partie de ce chapitre entend donner un aperçu des approches consacrées aux réactions inverses en théorie quantiques des champs en espace–temps courbe. Dans ce contexte, ces réactions inverses sont excercées par les champs quantiques matériels à l'espace–temps courbe classique. Les deux démarches que nous présentons sont connues sous les termes de gravité semi–classique et gravité stochastique.

Comme son nom le suggère, la théorie quantique des champs en espace–temps courbe tente à énoncer un formalisme bien défini des champs quantiques couplés à un champ gravitationnel classique. Ceci est évidemment une entreprise très difficile vu que les notions connues de la théorie des champs quantiques en espace de Minkowski sont fortement liées aux symétries présentes dans ce cas particulier. Par exemple, l'existence et l'unicité du vide de Minkowski est due aux symétries de Poincaré. Ce fait motive donc le choix d'un formalisme mathématique qui est basé sur l'algèbre des champs quantiques et non sur la représentation du vide et des états quantiques générale dans un espace de Hilbert. Par conséquent, nous présentons les bases de la théorie algébrique pour un champ scalaire réel: les axiomes de l'algèbre du champ basés sur les solutions classiques de la théorie, les fonctions de corrélations ainsi que la définition d'états quantiques et leur relation aux états vectoriels standards. Nous nommons plusieurs classes d'états importantes telles que les états de Hadamard, les vides adiabatiques et les états Gaussiens. À la suite, nous passons de cette approche covariante à une formule hamiltonienne qu'on obtient en choisissant des fonctions de test particuliers. Nous élaborons la théorie en utilisant un champs scalaire sur un espace–temps cosmologique qui bien reflète les propriétes des modèles considéres ultérieurement. En particulier, nous abordons les transformations de Bogoliubov qui donnent les relations entre des représentations différentes et dont certaines propriétés déterminent si les représentations sont unitairement équivalentes ou pas. Comme dans le cas classique considéré ci–dessus, l'impact possible des champs inhomogènes (et quantiques) sur le fond, c'est–à–dire l'espace–temps courbe, est estimé mineur.

Les approches de la gravité semi–classique et de la gravité (semi–classique) stochastique permettent d'intégrer ces effets de réactions inverses. Leur but ultérieur est de déduire des équations d'Einstein modifiées qui comprennent les effets des champs quantiques sur l'espace–temps courbes. Ces équations sont respectivement connus comme les équations d'Einstein semi–classiques et les équations d'Einstein–Langevin. Pour la première de ces deux méthodes, on com-

mence par calculer la valeur moyenne du tenseur énergie–impulsion dans un état quantique approprié. Le résultat fournit un nouveau terme de source pour le champ gravitationnel classique et définit ainsi les équations d'Einstein semi–classiques. La deuxième approche calcule une action effective pour la partie gravitationnelle du système en se servant des méthodes d'intégrations, et en déduit les équations d'Einstein–Langevin par principe de moindre action. Celles–ci comprennent les nouvelles sources de l'approche semi–classique mais le formalisme rajoute des termes dits stochastiques. Nous faisons référence à plusieurs modèles considérés dans ce contexte. À cause du formalisme mathématique lourd de ces théories et la difficulté de trouver des états susceptibles en théorie quantique des champs en espace–courbe, ces résultats se limitent aux configurations plutôt simplistes. Finalement, il faut aussi souligner que coupler un système quantique à un système purement classique est une procédure inconsistante.

II.5. Gravité et Cosmologie Quantique

Ce chapitre entend présenter plusieurs approches qui examinent des réactions inverses en gravité ou cosmologie quantique. Afin de réduire le nombre d'approches à considérer ici, nous nous limitons aux formalismes qui utilisent la masse de Planck inverse ou certains rapports de celle–ci comme paramètre perturbatif.

Le chapitre commence par les approches utilisées en géometrodynamique qui considèrent la masse de Planck inverse comme un paramètre de perturbation dans les équations de Wheeler–de Witt avec de la matière (c'est–à–dire les équations d'Einstein quantifiées). Ces approches recourent à une approche de Born–Oppenheimer dans une première étape en employant une certaine forme pour les solutions quantiques du problème et qui sont nécessaires pour son évaluation. Malheureusement, les équations résultantes restent si complexes qu'il faut recourir à une fonction d'approche semi–classique pour pouvoir avancer. Nous remarquons également qu'il est possible d'identifier un paramètre de temps en se servant des équations de Hamilton–Jacobi classiques. Toutes ces approches sont toutefois basées sur des approximations semi–classiques qui de façon conséquente réduisent le domaine d'application de la théorie. En particulier, cela empêche son utilisation pour des systèmes purement quantiques.

Nous faisons aussi référence à des études poursuivies en gravitation quantique à boucles qui utilisent également l'approche de Born–Oppenheimer. Leur but est surtout de dériver une théorie quantique des champs en espace–temps courbe à partir de cette approche de la gravitation quantique. Une des difficultés initialement rencontrées dans ces études est due à la non–commutativité de certaines variables, particulièrement les champs du secteur gravitationnel qui sont couplés aux champs de matière. Cela nécessite une extension de l'approche de Born–Oppenheimer qui s'applique seulement aux cas commutatifs dans ce sens précis. Dans ce contexte, Stottmeister et Thiemann ont exploité la théorie des perturbations spatio–adiabatique qui est a priori adaptée à une application en gravité quantique. Néanmoins, leurs résultats restent sur un niveau formel en raison de la structure nécessairement compliquée d'une théorie de gravité quantique.

Cependant, il est possible d'appliquer la théorie des perturbations spatio–adiabatiques aux

systèmes cosmologiques, qui sont plus faciles à analyser en termes de structure mathématique. Bien que des difficultés similaires aux problèmes des théories quantiques des champs sur un espace-temps courbe se posent ici, les réductions de symétrie (avec des perturbations) permettent néanmoins une analyse des effets de réactions inverses dans ce contexte. En particulier, lorsque l'on considère la théorie des perturbations cosmologiques standard, il est nécessaire d'utiliser la théorie des perturbations spatio–adiabatiques car, pour les mêmes raisons que celles mentionnées ci–dessus, il n'est pas possible d'appliquer l'approche de Born–Oppenheimer.

II.6. Systèmes Quantiques Couplés

Ce dernier chapitre de la partie II entend énoncer l'idée et les bases de l'approche de Born–Oppenheimer usuelle employée en physique des molécules ainsi que les bases de la théorie des perturbations spatio–adiabatiques selon Panati, Spohn et Teufel. En particulier, nous abordons les limites de la théorie de Born–Oppenheimer et expliquons pourquoi la théorie spatio-adiabatique est une extension appropriée qui permet non seulement une extension constructive à des ordres de perturbation plus élevés mais est également applicable à une classe bien plus large de systèmes. Après une introduction à la théorie spatio–adiabatique selon Panati, Spohn et Teufel, en particulier aux conditions et aux étapes de construction explicites, nous discutons le caractère itératif de la théorie et prouvons que la théorie est cohérente. De plus, nous donnons de manière très explicite les formules algébriques nécessaires pour effectuer la construction jusqu'au deuxième ordre dans les perturbations. Enfin, nous appliquons la théorie à un exemple de deux oscillateurs couplés et réalisons le schéma jusqu'au second ordre.

Le chapitre commence par reproduire l'approche de Born–Oppenheimer pour une molécule simple. En partant de l'équation de Schrödinger stationnaire et en utilisant le petit rapport de masse entre les électrons et les noyaux, nous obtenons un opérateur hamiltonien perturbatif pour ce modèle. En considérant les noyaux comme des quantités classiques, la théorie donne un opérateur hamiltonien effectif pour les électrons, qui dépend toutefois de manière paramétrique des variables nucléaires. En supposant que ce système a des solutions paramétriques, nous pouvons dériver un hamiltonien effectif pour le noyau en le projetant sur ces solutions électroniques. Pour cela, il était nécessaire d'utiliser un état quantique qui a la forme d'un produit. La réduction de cet opérateur à l'ordre zéro ou au premier ordre des perturbations réfère à l'approche de Born-Oppenheimer.

Évidemment, cette théorie est fondée sur l'usage d'un état quantique spécifique et une extension aux ordres plus élévés dans les perturbations n'est pas possible. Dans une première étape, cela nous incite à recourir à une approximation, également basée sur le paramètre de perturbation employé ci–dessus, mais qui ne nécessite pas un état quantique spécifique. Ce sont donc les équations algébriques des opérateurs qui définissent cette théorie adiabatique et dynamique de premier ordre. Quoique cette théorie soit plus générale que l'approche de Born–Oppenheimer usuelle, elle est toujours limitée au premier ordre dans les perturbations adiabatiques.

Un autre défaut de cette théorie, comme pour l'approche de Born–Oppenheimer, est lié au

fait que ces théories sont basées sur l'existence d'un spectre simultané des opérateurs de couplage du système lent. Plus précisément, elles s'appuient sur le fait que les opérateurs des positions des noyaux commutent. Cela limite évidemment l'applicabilité de l'approche et notamment empêche son usage pour les systèmes en cosmologie inhomogène qu'on voudrait considérer dans une étape ultérieure. Pour cela, on présente l'exemple d'une particule de Dirac couplée à un champ électromagnétique classique. La forme de l'hamiltonien motive à considérer une théorie quantique du système rapide "sur" l'espace des phases du système lent.

Avant de passer à une telle approche, nous remarquons que la théorie adiabatique–temporelle est en fait comprise dans la théorie spatio–adiabatique que nous allons aborder. Plus précisément, il faut imaginer le temps comme un paramètre extérieur et la dérivée temporelle apparente dans l'équation de Schrödinger comme une perturbation de l'hamiltonien qui lui–même dépend du temps. Finalement, nous faisons aussi référence à une approche qui utilise des états cohérents pour lever la restriction aux modèles avec des couplages commutatifs. Nous démontrons les difficultés de cette procédure et soulignons que la théorie spatio–adiabatique est plus flexible, simple et directe.

Avec ces résultats, nous commençons par la suite à énoncer les bases de la théorie des perturbations spatio–adiabatiques. La première partie consiste à renouveler les idées sous–jacentes à la quantification de Weyl qui utilise des transformations de Fourier pour établir une quantification des éléments de Weyl ainsi que de chaque opérateur qu'on peut en déduire. Cela mène à une représentation des opérateurs comme opérateurs intégraux si appliqués à une fonction d'onde. Le noyau d'un tel opérateur est particulièrement intéressant car il détermine uniquement, dès qu'un ordre des opérateurs est fixé, l'effet de cet opérateur. En effet, il est possible de retirer la mécanique quantique entièrement sur l'espace des phases sans faire référence à une représentation sur un espace de Hilbert. Au lieu de travailler avec des opérateurs algébriques représentés sur un espace d'états quantiques, on effectue donc les calculs dans une algèbre des fonctions sur l'espace des phases. Naturellement, le produit d'opérateurs se traduit en un produit non–commutatif nommé "produit étoile". La théorie résultante est la mécanique quantique de l'espace des phase, et elle est physiquement équivalente à l'approche usuelle. Comme en mécanique quantique standard, il est possible de récupérer la mécanique classique dans la limite $\hbar \to 0$, mais ici la relation est plus évidente car on travaille déjà sur l'espace des phases. À l'avenant, le produit étoile a la forme d'une série entière en $\hbar$.

Revenons maintenant à la théorie des perturbations spatio–adiabatiques pour les systèmes couplés quantiques admettant un paramètre perturbatif qui caractérisent deux échelles énergétiques différentes du système. Dans un tel système, il est souvent possible de redimensionner un des variables du système lent en multipliant par le paramètre perturbatif. Cette procédure par contre redimensionne aussi le produit étoile si on considère la théorie sur l'espace des phases. Il en résulte donc une théorie perturbative au niveau des équations de mouvement si on développe le produit étoile respectivement. L'idée de base de cette théorie est donc comme suivant: On divise le système dans une partie "lente" et une partie "rapide" afin de retirer la théorie quantique du système lent à l'espace des phases. L'identification d'un paramètre perturbatif et la redimension d'une des variables lentes aboutissent à une théorie perturbative mais purement quantique. Le système rapide est cependant toujours représenté sur un espace de Hilbert et a la forme d'une mécanique quantique usuelle. Le calcul correspondant s'appelle le calcul pseudo–différentiel à

valeurs d'opérateurs et représente une extension directe du calcul pseudo–différentiel scalaire. Nous donnons une petite introduction à ce calcul focalisée sur les aspects importants par la suite.

Avec ces informations, nous sommes donc prêts à introduire la théorie des perturbations spatio–adiabatiques. À cet égard, nous suivons les définitions et le schéma de Panati, Spohn et Teufel. La première étape consiste en présenter les quatres conditions que chaque modèle est obligé de satisfaire afin que le schéma soit applicable. Puis, la théorie se divise en trois étapes: La construction d'un projecteur, d'un opérateur unitaire et un hamiltonien effectif. Ce dernier n'agit que sur le système lente mais inclut les réactions inverses du système rapide. Le schéma est constructif et permet donc d'approcher la dynamique originale à une erreur de l'ordre souhaité près. Plus précisément, ce formalisme construit un hamiltonien effectif dont le problème des valeurs propres est considérablement plus simple à résoudre mais dont les solutions approchent les vraies solutions à une petite erreur près.

Pour obtenir les équations de mouvement quantique qui déterminent les solutions à un erreur ε^{n+1} près il faut poursuivre la démarche du schéma jusqu'à l'ordre n. Nous montrons dans ce chapitre que le schéma est cohérent en soi et qu'il produit des opérateurs bien définis. Puis, nous considérons les étapes de construction jusqu'à l'ordre deux plus en détail et cela pour des systèmes d'une forme que nous rencontrerons à la suite. Plus concrètement, la partie rapide de ces systèmes spécifiques est donnée par un nombre fini ou infini d'oscillateurs harmoniques dont la masse ou la fréquence dépend des variables lents. Nous utiliserons donc ces formules à nombreux endroits par la suite du manuscrit.

Enfin, la dernière partie de ce chapitre entend appliquer le formalisme spatio–adiabatique à un simple exemple comprenant deux oscillateurs dont l'oscillateur rapide est harmonique. Le sous–système anharmonique a la forme d'un oscillateur anharmonique. Nous suivons le schéma jusqu'au deuxième ordre et dérivons le projecteur, le symbole unitaire et l'hamiltonien effective. Nous récupérons les résultats de Born et Oppenheimer à l'ordre zéro et des perturbations quantiques à l'ordre deux. Grâce au spectre discret de l'opérateur non–perturbé, on peut d'employer la théorie des perturbations usuelle en mécanique quantique.

III. Cosmologie Quantique et Réactions Inverses

III.7. Cosmologie Homogène et Isotrope

La troisième partie de cette thèse entend présenter l'application de la théorie des perturbations spatio–adiabatiques à des modèles divers en cosmologie. Ce chapitre commence par considérer un modèle simple d'une cosmologie spatialement homogène et isotrope. Le modèle contient une partie géometrique paramétrisée par le facteur d'échelle et son moment conjugé et une constante cosmologique ainsi qu'un champ scalaire réel, également homogène et isotrope. Ce dernier est plus précisément un champ de Klein–Gordon avec une masse m et un potentiel quadratique.

Dans une première étape, nous passons à un formalisme hamiltonien par une transforma-

tion de Legendre pour pouvoir appliquer le schéma. D'ailleurs, nous introduisons un nouveau pair canonique pour le système géométrique qu'on peut identifier avec une variable de triades et son moment conjugé. Puis, le schéma spatio–adiabatique exige qu'une quantification soit formellement effectuée pour le système matériel qui, comme annoncé avant, est un simple oscillateur harmonique dont la masse dépend de la géométrie. Avec les nouvelles variables, la partie géometrique obtient la forme d'un oscillateur inverse.

Afin de pouvoir appliquer la théorie spatio–adiabatique à ce modèle, il est nécessaire de vérifier les conditions énoncées au dernier chapitre. Grâce au spectre discret de l'oscillateur harmonique représentant le champ de Klein–Gordon, il est simple de prouver que le modèle admet des lacunes non–nulles entre ses bandes d'énergie, ce qui est une des prémisses de la théorie. Vu qu'il s'agit un modèle avec un nombre de degrés de liberté fini (il y'en a que deux), la première condition est satisfaite sans autre action parce que l'espace de Hilbert a naturellement la forme d'un produit tensoriel. Les deux conditions restant concernent la forme de l'hamiltonien du système. En particulier, ils exigent que la fonction symbolique de l'hamiltonien ait des valeurs dans l'espace des opérateurs bornés sur l'espace de Hilbert de la matière ainsi que la fonction symbolique soit polynomialement bornée vis–à–vis du moment cinétique et bornée vis–à–vis de la configuration de la géométrie. Cela nous oblige de définir un hamiltonien auxiliaire pour pouvoir garantir la convergence de la série perturbative. Cet hamiltonien auxiliaire satisfait la totalité des quatres conditions mais ne correspond que sur un domaine restreint de l'espace des phases de la géométrie à l'hamiltonien original.

Ces préparations permettent donc l'application du schéma et nous construisons le symbole d'un projecteur et d'un opérateur unitaire jusqu'à l'ordre un. En effet, cela suffit pour obtenir un hamiltonien effectif à l'ordre deux. Nous trouvons qu'à l'ordre zéro le résultat correspond toujours à la solution de l'approche de Born–Oppenheimer. Il s'agit d'un oscillateur inverse avec une énergie du point zéro non–nulle mais constante. Le premier ordre est nul alors que le deuxième ordre donne plusieurs corrections à l'ordre zéro. Cette perturbation contient non seulement un terme potentiel non–polynomiale mais aussi une contribution cinétique, également avec une dépendence non–polynomiale de la configuration de la géométrie. En se limitant à l'ordre zéro, nous pouvons utiliser les solutions connues de l'oscillateur inverse pour résoudre la contrainte. Ces solutions ne sont pas de carré sommable et le spectre consiste en la ligne réelle entière, donc il s'agit d'un spectre continu. Cele nous êmpeche d'employer la théorie des perturbations usuelle en mécanique quantique. Même pire, nous observons que les perturbations d'un spectre continu sont très instables. Nous devons donc reporter la recherche de solutions à un travail ultérieur.

Enfin, ce chapitre entend discuter deux propriétés de l'hamiltonien effectif obtenu ici et qui se posent également dans les chapitres suivants. Premièrement, il faut souligner qu'il s'agit d'une *contrainte* et non d'un hamiltonien physique. L'existence d'un vrai hamiltonien borné par le bas est toutefois nécessaire pour la validité de l'équipartion de l'énergie. Par conséquent, il n'est plus possible d'associer une grande masse avec une dynamique lente et donc la distinction système lent – rapide se périme. Il est néanmoins possible d'utiliser la contrainte classique pour identifier des régions dans l'espace des phases pour lesquelles la géométrie représente le système lent tandis que le champ scalaire représent la partie rapide.

Deuxièmement, la partie de la contrainte hamiltonienne effective de l'ordre deux contient des fonctions non–polynomiales de la variable géométrique. Bien que la quantification de Weyl de

ces fonctions dans sa forme intégrale ne pose pas de problème en soi, trouver un domaine admissible et des solutions de la contrainte est difficile. Ce problème sera encore aggravé par la suite, car les modèles inhomogènes produisent des fonctions qui ne sont pas polynomiales en ce qui concerne les moments conjugés. Pour cela, nous montrons qu'il est pourtant possible d'identifier des domaines susceptibles dans plusieurs cas particuliers.

III.8. Cosmologie Inhomogène avec Poussière

Ce chapitre est le premier de deux dans lesquels nous considérons des modèles cosmologiques inhomogènes. Comme précédemment, ces modèles contiennent une partie purement spatialement homogène et isotrope de la géométrie (et éventuellement de la matière), mais sont complétés par des perturbations linéaires des champs cosmologiques. Dans tous les modèles, nous considérons des degrés de liberté géométriques ainsi qu'un champ scalaire réel, mais selon la commodité, nous divisons les secteurs homogènes et inhomogènes de manière différente et effectuons des transformations des champs si nécessaire. Le point commun de tous ces modèles est qu'ils prennent la forme d'une théorie quantique des champs sur un espace–temps courbe dans le cadre de la théorie des perturbations spatio–adiabatiques. Le fond est représenté par des degrés de liberté homogènes et isotropes. Étant donné cette forme, le schéma spatio–adiabatique exige que chaque théorie quantique des champs soit unitairement équivalent dans le sens usuel en théorie quantique des champs pour chaque configuration des variables homogènes. Comme nous l'avons montré, ceci n'est pas le cas a priori et le schéma ne serait donc pas applicable. Heureusement, il est possible de résoudre ce problème grâce à certaines transformations des champs et des variables homogènes. Ce chapitre commence par exposer les raisons pour lesquelles la théorie spatio–adiabatique ne peut pas être appliquée en premier lieu. Nous définirons ensuite une classe générale de transformations qui permettent une application suivante. Par la suite, nous appliquerons une telle transformation à l'un des modèles inhomogènes avant d'exécuter la théorie des perturbations spatio–adiabatiques.

Dans une première étape, nous choisissons un modèle avec une partie géométrique et un champ scalaire réel spatialement homogène et isotrope, ainsi que des perturbations du champ scalaire. D'ailleurs, le modèle contient, par facilité, un champ de poussière qui sert à déparamétriser la thèorie. Nous récuperons donc un hamiltonien physique. Dans ce cas, l'action ainsi que l'hamiltonien de la partie perturbative du modèle dépendent du champ et de son moment conjugé de manière quadratique mais également de la géométrie homogène, plus précisément du facteur d'échelle. Comme les hypersurfaces spatiales du modèle correspondent à des tores trois–dimensionnelle et compacts, une transformation de Fourier des champs montre que le modèle coïncide avec un ensemble dénombrable d'oscillateurs harmoniques dont les fréquences dépendent du facteur d'échelle.

Puis, il s'avère que les représentations de Fock "naturelles" de la théorie quantique des champs associée ne sont pas équivalents l'un à l'autre pour différentes valeurs du facteur d'échelle. En plus de cela, nous montrons que le vide d'une des représentations ne constitue pas un état normalisable vis–à–vis d'une des autres représentations, même pas pour des valeurs du facteur

d'échelle qui sont très proches. C'est la condition de Hilbert–Schmidt qui est violée. Pareillement, la théorie ne nous permet pas de représenter l'opérateur du moment conjugé de la géométrie homogène comme un opérateur bien défini dans les espaces de Fock. Nous montrons que l'opérateur du moment appliqué au vide donne un résultat non normalisable. Cependant, il est facile d'identifier la cause de ces anomalies: les fréquences et particulièrement leur contribution qui contient l'opérateur de Laplace–Beltrami dépend du facteur d'échelle. Une fois que cette dépendance est supprimée, les théories quantiques des champs admettent des représentations équivalents.

Cela nous conduit à chercher des transformations susceptibles qui sont capables de supprimer cette dépendence. A cet égard, il faut noter que la canonicité de toutes les variables impliquées doit être préservée, puisqu'en fin de compte nous voulons aussi quantifier les variables homogènes. Cela exlut par exemple d'employer des transformations pour le secteur inhomogène générique qui dépendent des variables homogènes. Il semble très difficile de trouver une telle transformation qui soit exactement canonique. Nous suivons donc une approche approximative et exigeons seulement que les transformations soient canoniques jusqu'au deuxième ordre dans les champs perturbatifs. Cela est raisonnable puisque de toute façon la théorie coupe l'hamiltonien après cet ordre.

L'investigation du potentiel symplectique nous permet finalement d'énoncer une classe de transformations qui est qualifiée pour résoudre les problèmes mentionnés ci–dessus (c'est–à–dire elle lève la dépendence aux variables homogènes du terme associé à l'opérateur Laplace–Beltrami) et garantit en outre que l'opérateur hamiltonien transformé reste bien défini. Muni de ces transformations, nous sommes prêtes à appliquer la théorie des perturbations spatio–adiabatiques.

Par la suite, nous considérons un modèle avec une partie géométrique spatialement homogène et isotrope, une constante cosmologique, un champ de poussière pour déparamétriser la théorie ainsi qu'un champ scalaire inhomogène du type Klein–Gordon. Contrairement au modèle précédent, ce modèle ne contient pas de mode homogène du champ scalaire. Dans le modèle précédent, ce mode était principalement utilisé pour démontrer la généralité des transformations. Puisque le champ de poussière déparamétrise déjà la théorie, le champ scalaire homogène peut être simplement attribué à la partie inhomogène. Avec ce modèle, nous considérons ensuite l'application de la théorie des perturbations spatio–adiabatiques.

Le schéma procède de manière très similaire comme pour les exemples précédents, avec la seule différence que le simple oscillateur "rapide" soit remplacé par un nombre infini mais dénombrable d'oscillateurs avec des fréquences différentes et qui dépendent toujours de la géométrie homogène. Comme précédemment, nous sélectionnons un état dans l'espace de Fock pour calculer le symbole d'un projecteur, d'un opérateur unitaire ainsi qu'un hamiltonien effectif jusqu'à l'ordre deux des perturbations spatio–adiabatiques. Ce dernier agit sur la géométrie homogène et inclut les effets des réactions inverses de l'état de Fock choisi avant. L'ordre zéro de ce dernier symbole reproduit le résultat de l'approche de Born–Oppenheimer. Cette partie contient la contrainte hamiltonienne usuelle d'une géométrie homogène et isotrope (avec une constante cosmologique) ainsi que l'énergie des bandes d'énergie de l'état de Fock choisi. Le symbole d'ordre un est nul tandis que le deuxième ordre donne un résultat non–trivial. Comme pour les exemples précédents, celui–ci contient des fonctions de la géométrie homogène non–polynomiale. De surcroît, ce terme dépend de *toutes* les bandes d'énergie de tous les états de Fock possible. Il semble donc possible, à première vue, que cet hamiltonien ne converge pas. Heureusement, les bandes contribuent d'une

manière convergente. De plus, les carrés des fonctions de fréquence sont définis positifs comme on peut s'y attendre dans une théorie quantique des champs standard.

Néanmoins, trouver un domaine de cet opérateur ou bien des solutions une fois qu'il a été quantifié par la méthode de Weyl sera difficile. Nous reporterons cette analyse à une recherche ultérieure. Nous notons cependant que le théorème du chapitre précédent sur l'existence de domaines pour les opérateurs non–polynomiaux pourrait être utile.

III.9. Cosmologie Inhomogène et Invariante de Jauge

Ce chapitre représente la partie principale de ce manuscrit. Tous les exemples précédents peuvent être considérés comme une préparation à l'analyse du modèle suivant. En particulier, ce chapitre entend étudier la théorie des perturbations cosmologiques standard qui est fréquemment utilisée, notamment pour comparer les modèles cosmologiques aux données mesurées. Comme pour les modèles précédents, nous considérons à nouveau une théorie consistante d'une composante géométrique homogène et isotrope, une constante cosmologique, et cette fois également un mode homogène et isotrope d'un champ scalaire du type Klein–Gordon. La partie inhomogène du modèle comporte les perturbations de la géométrie ainsi que les perturbations du champ scalaire réel. Contrairement à l'exemple précédent, ce modèle ne comporte pas de champ de poussière déparamétrisant et la théorie est donc contrainte.

Sans ce champ de poussière, il n'y pas de coordonnées privilégiées mais la répartition en mode homogène et inhomogène a brisé la covariance de la théorie. Il est possible de rétablir cette covariance à l'ordre linéaire des perturbations en utilisant des variables invariantes de jauge dans le secteur inhomogène. Premièrement, il est utile de décomposer les champs inhomogènes de cette théorie en une partie scalaire, vectorielle et tensorielle en fonction de leur comportement sous les rotations de $SO(3)$. Puis, nous pouvons introduire des variables invariantes de jauge indépendamment pour chacun de ces secteurs. Dans le secteur scalaire, il s'agit du champ de Mukhanov–Sasaki bien connu et les perturbations tensorielles sont déjà invariantes de jauge. Le problème avec les transformations de ce genre est qu'elles impliquent les variables homogènent et donc brisent la canonicité du système. Dans le cas où on considère le fond comme fixé ceci ne pose pas de problème, mais dans un formalisme où les variables homogènes sont considérées comme dynamiques et soumises à une quantification ultérieurement, c'est inadmissible. Comme dans l'exemple précedent, il faut envisager des transformations plus génériques qui tiennent compte du secteur homogène. Par ailleurs, ces transformations doivent prévenir les anomalies rencontrées au dernier chapitre qui sont reliées à la condition de Hilbert–Schmidt. Une dernière condition est que le nouvel hamiltonien ne contienne que des termes qui soient bien définis sur les espaces de Fock correspondants.

Dans le contexte de ce modèle spécifique, nous pouvons nous servir de la littérature existante. En effet, dans l'approche hybride en cosmologie quantique, de telles transformations ont déjà été traitées et elles sont explicitement applicables à notre modèle. Ces transformations contiennent les transformations usuelles pour obtenir des champs perturbatifs invariants de jauge,

par exemple les transformation de Mukhanov–Sasaki, mais les complètent par des transformations des variables homogènes. Ces dernières sont elles–mêmes du second ordre dans les perturbations cosmologiques et se traduisent par des termes supplémentaires de second ordre dans la nouvelle contrainte hamiltonienne de la théorie. En particulier, la nouvelle contrainte garde formellement sa forme mais la masse originale du champ de Klein–Gordon est remplacée par une fonction compliquée des variables homogènes – une nouvelle masse effective.

Avec ces transformations, il est possible d'appliquer le schéma spatio–adiabatique. Une analyse des contraintes montre que la seule contrainte non–triviale restante consiste en la partie homogène usuelle de la théorie cosmologique plus des contributions scalaires et tensorielles de second ordre. Les deux dernières sont comme avant quadratique dans leurs variables et leurs moments conjugés, mais les masses dépendent maintenant du secteur homogène. Dans une première étape, le schéma quantifie les champs inhomogènes menant formellement à une théorie quantique des champs en espace courbe. Cette théorie contient la partie scalaire de Mukhanov–Sasaki ainsi que deux modes tensoriels. Nous appliquons le schéma de la même manière que dans le chapitre précédent. Il en résulte une contrainte hamiltonienne (d'ordre deux dans les perturbations spatio–adiabatiques) qui nécessite une analyse plus approfondie. En effet, l'hamiltonien comprend des termes qui sont d'un ordre plus élevé ce qui est dû à notre partition de l'hamiltonien dans une première étape. Après cette analyse et la suppression de termes trop élévés, nous arrivons au résultat final. Celui–ci contient la partie usuelle complètement homogène et isotrope ainsi que l'énergie de l'état de Fock choisi au début du schéma. Il faut noter que cette énergie est une fonction compliquée du secteur homogène car elle contient des masses effectives. À l'ordre deux, la contrainte hamiltonienne dépend de toutes les énérgies des états de Fock, plus précisément des énergies de la partie scalaire. La partie tensorielle ne contribue pas aux effets de réactions inverses dans ce modèle. Comme pour l'exemple précédent, on peut montrer que les contributions convergent mais seulement si les masses effectives sont définies positives.

Cependant, ces carrés de masse ne sont pas nécessairement positifs. Il s'agit des fonctions sur l'espace des phases homogène qui peuvent prendre des valeurs négatives sur certains domaines. Ceci est particulièrement inquiétant car des champs de carré de masse négatives sont soumis à des instabilités tachyoniques. Par la suite, nous proposons donc plusieurs stratégies pour gérer ces problèmes. Entre autres, nous proposons d'étudier plus en détail les transformations effectuées ci–dessus et éventuellement de trouver d'autres transformations qui ne conduisent pas aux carrés de masse indéfinis. En fait, nous nous sommes limités à une transformation particulière. Une autre possibilité consiste à effectuer une transformation ou un plongement canonique supplémentaire dans l'espace de phase homogène qui est conçue exactement de manière à ce que les carrés de masse deviennent définis positifs. En effet, nous avons déjà appliqué cette stratégie au dernier chapitre. Ressemblablement, nous poursuivons cette tactique ici.

Pour ce faire, nous considérons les deux paires canoniques du secteur homogène et les transformons de sorte que les carrés de masse soient manifestement positifs. Ce faisant, l'une des variables doit être restreinte à l'union de deux intervalles compacts. L'application suivante du schéma spatio–adiabatique génère une contrainte hamiltonienne fondamentalement différent, en particulier cette fois–ci les modes tensoriels sont également impliqués en ce qui concerne les réactions inverses d'ordre deux. Cela n'est pas surprenant puisqu'une transformation canonique classique peut très bien conduire à une théorie quantique différente. Seulement l'expérience peut déter-

miner laquelle des deux théories est l'importante. Néanmoins, ce modèle nécessite une révision: En effet, la quantification de Weyl ainsi que le produit étoile ne sont définis que pour des modèles avec un espace des phases de la forme $T^*\mathbb{R}^n$. Les variables fondamentales doivent donc assumer toute valeur réelle. Ce n'est évidemment plus le cas et les formules de Weyl ne sont conséquemment plus applicables. Par la suite, nous examinons donc deux solutions possibles à ce problème mais qui apportent aussi des difficultés. Cependant, une fois ces problèmes levés, nous disposons d'une contrainte hamiltonienne bien définie qu'il reste à quantifier dans une dernière étape. De nouveau, nous devons reporter la recherche d'un domaine de définition et des solutions possibles à un projet ultérieur.

Dans la dernière section de ce chapitre, nous revenons à la question de savoir comment une division en un secteur lent et un secteur rapide pourrait se présenter pour les modèles inhomogènes. Nous faisons référence à l'idée d'associer une masse lourde aux variables homogènes et une masse petite aux modes inhomogènes. Pour ce faire, il faut diviser le torus trois–dimensionel spatial en petits segments et définir de nouvelles variables en fonction de ceux–ci. Ces segments engendrent un nombre dénombrable de degrés de liberté et peuvent en fait être associés à une petite masse. Dans une dernière étape, ces variables peuvent être associées aux modes du champ original en utilisant une transformation unitaire. Nous avons étudié cette question plus en détail dans l'un des articles connexes.

IV. Conclusion et Perspectives d'Avenir

IV.10. Conclusion

Dans cette thèse, nous avons abordé la question des réactions inverses en cosmologie en nous concentrant sur le problème de ces effets en cosmologie quantique inhomogène. Plus précisément, nous avons considéré la question de savoir si et dans quelle mesure les champs quantiques et inhomogènes influencent l'évolution globale d'un Univers quantique. Pour trouver une réponse à cette question, nous avons recouru au formalisme des perturbations spatio–adiabatiques introduit par Panati, Spohn et Teufel. De surcroît, nous avons étendu ce schéma de manière appropriée afin d'inclure des modèles de théorie quantique des champs. Ce chapitre avant–dernier entend donner un résumé et une conclusion de nos résultats.

Nous avons commencé avec un historique des développements de la physique au cours du 20e et 21e siècles qui ont conduit à la construction du modèle physique contemporain comprenant la relativité générale ainsi que le modèle standard de la physique des particules. Relié aux données de mesure cosmologique de haute précision, ce modèle suggère que l'Univers a toujours été en expansion tout au long de son histoire connue et qu'il était donc très chaud et dense pendant ses premiers moments. Une théorie de l'Univers primordial devrait donc faire appel aux méthodes de la théorie quantique des champs en espace–temps courbe ou à la gravité quantique. Afin de progresser dans l'étude de l'Univers primordial dans le cadre de ces deux théorie très com-

plexes, il est possible d'employer des schémas approximatifs et d'exploiter les symétries connues du système. Cela conduit à la théorie des perturbations cosmologiques et quantiques qui devrait être pertinente lorsque les inhomogénéités du système sont faibles par rapport aux contributions purement homogènes du système. La procédure habituelle de ces approches consiste à propager les champs quantiques et inhomogènes sur un fond quantique effectif préalablement fixé. Ensuite, les réactions inverses des champs quantiques inhomogènes sur l'évolution globale du fond sont négligées.

Bien entendu, le problème de négliger les réactions inverses joue également un rôle dans les modèles classiques de l'Univers, et nous avons passé en revue les méthodes qui consistent à inclure ces effets. Pourtant, ces nombreuses approches n'ont pas encore trouvé de réponse concluante. La même question se pose dans les théories semi–classiques comme la théorie quantique des champs en espace–temps courbe. Nous avons considéré les approches de la gravité semi–classique et de la gravité stochastique (semi–classique) qui abordent le problème des réactions inverses. Dans les deux cas, il faut d'abord trouver des états quantiques admissibles pour évaluer la valeur moyenne du tenseur d'énergie–impulsion de la matière afin de trouver, dans une deuxième étape, des solutions aux équations d'Einstein classiques modifiées qui incluent ces termes (et éventuellement d'autres contributions "stochastiques") comme sources supplémentaires. En raison des difficultés génériques d'identification des états appropriés qui conduisent à une valeur moyenne bien définie du tenseur d'énergie–impulsion dans un espace–temps génériquement courbé, cette entreprise n'est pas triviale et n'est réalisée que pour certains contenus de matière (plutôt simplistes). De même, la deuxième étape, qui consiste à trouver des solutions aux équations d'Einstein modifiées, s'avère complexe car il faut faire face à des problèmes de stabilité. D'ailleurs, d'un point de vue conceptuel, l'approche semi–classique ne peut pas représenter la théorie finale.

Pour aborder une discussion purement quantique du problème, nous avons considéré les approches connues en gravité et en cosmologie quantique. Nous nous sommes concentrés sur les idées qui utilisent une expansion perturbative dans l'inverse de la masse Planck et, plus précisément sur les méthodes de type Born–Oppenheimer. Pour obtenir des résultats pertinents, la plupart de ces approches emploient cependant une limite semi–classique ou restent sur un niveau formel. Pour resoudre ces problèmes et pour surmonter les difficultés usuelles de l'approche de Born–Oppenheimer, nous suggérons d'utiliser le nouveau formalisme des perturbations spatio–adiabatiques de Panati, Spohn et Teufel. Par la suite, nous donnons une introduction approfondie à cette théorie et fournissons tous les outils mathématiques nécessaires.

Le premier exemple auquel nous avons appliqué ce formalisme perturbatif consiste en un oscillateur harmonique rapide couplé à un oscillateur anharmonique et lent. Le couplage s'effectue par l'énergie potentielle des deux oscillateurs. Le paramètre de perturbation adiabatique est défini comme le rapport de leurs masses. Bien que le modèle ne comprenne que deux dégrés de liberté, ce qui permet normalement une application directe du formalisme, nous avons modifié l'opérateur hamiltonien pour assurer la convergence de la série perturbative. Puisque les calculs restent valables localement, nous avons tout de même continué à utiliser l'hamiltonien original. L'hamiltonien effectif résultant du schéma spatio–adiabatique comprend l'approche usuelle de Born–Oppenheimer à l'ordre zéro et des contributions supplémentaires à l'ordre deux. Nous avons pu résoudre le problème quantique de cet opérateur en utilisant la théorie des perturbations en mécanique quantique standard et avons donc implémenté des réactions inverses de l'oscillateur

rapide au problème de l'oscillateur lent.

En tant que modèle cosmologique quantique, nous avons abordé une cosmologie homogène et isotrope avec une constante cosmologique et couplée à une particule scalaire massive à valeur réelle. Le secteur géométrique apparaît naturellement comme le système redimensionné par un petit paramètre perturbatif qui est donné par le rapport entre la constante de couplage gravitationnelle et la constante de couplage de la matière. Puisque le système est contrainte, l'attribution habituelle des secteurs rapides et lents due au théorème d'équipartion échoue. Néanmoins, nous pouvons identifier des régions dans l'espace des phases pour lesquelles cette interprétation est restaurée. Comme pour l'exemple précédent, nous sommes en mesure de construire une contrainte hamiltonienne effective quantique pour la géométrie, y compris les effets des réactions inverses du champ scalaire. La théorie résultante à l'ordre zéro est un oscillateur inverse qui a un spectre réel continu. Malheureusement, cela implique que la théorie standard des perturbations en mécanique quantique pour évaluer l'hamiltonien effectif du second ordre n'est plus disponible, et nous laissons l'analyse plus approfondi du problème spectral pour de la recherche future.

Le troisième modèle dans cette thèse applique le formalisme adiabatique à une géométrie purement homogène et isotrope, couplée à un champ de Klein–Gordon inhomogène et à un champ de poussière. Techniquement, le schéma nous oblige d'abord à considérer une théorie quantique des champs sur un espace–temps courbe classique. Cependant, nous montrons que ces théories pour différentes configurations de la géométrie sont physiquement inéquivalentes dans le sens où la condition de Hilbert–Schmidt est violée. Nous trouvons une solution pour cela en employant des transformations pour l'ensemble du système canonique qui sont canoniques jusqu'au second ordre dans les perturbations cosmologiques, et qui ont été précédemment introduites dans l'approche hybride à la cosmologie quantique. L'application du schéma jusqu'au second ordre perturbatif nous fournit alors un hamiltonien effectif pour le secteur homogène incluant les réactions inverses du champ de Klein–Gordon quantique inhomogène. À l'ordre zéro, nous retrouvons la contrainte homogène usuelle en cosmologie ainsi qu'une contribution d'énergie potentielle effective provenant des bandes d'énergie du champ de Klein–Gordon. Cela correspond en fait au résultat standard de Born–Oppenheimer. Cependant, la contrainte effective du second ordre va au–delà et produit des corrections qui dépendent en partie de toutes les bandes d'énergie possibles du champ de Klein–Gordon. En particulier, il y a des effets provenant du vide de la théorie quantique des champs. Ces contributions convergent mais dépendent de manière non–polynomiale à la fois de la configuration géométrique et de son moment conjugué.

Le dernier modèle est une cosmologie inhomogène qui se compose, d'une part, du secteur homogène et isotrope habituel de la géométrie et d'un champ scalaire massif de Klein–Gordon, et d'autre part, des champs de perturbations linéaires invariants de jauge. Ce système est complètement contraint et nous effectuons donc une analyse de Dirac afin d'obtenir les contraintes pertinentes. Avec les transformations qui empêchent la condition de Hilbert–Schmidt d'échouer, nous obtenons une seule contrainte hamiltonienne. Sa contribution d'ordre zéro a la forme standard de la contrainte cosmologique purement homogène, tandis que le second ordre consiste en deux parties associées au champ de Mukhanov–Sasaki et aux gravitons. Les deux champs inhomogènes ont la forme d'un champ scalaire minimalement couplé dont les masses effectives sont des fonctions indéfinies des degrés de liberté homogènes. Nous appliquons le schéma adiabatique et obtenons une contrainte effective pour la géométrie homogène et le système de Klein–Gordon

qui inclut réactions inverses des perturbations de Fock. A l'ordre zéro, nous récupérons les contributions usuelles de Born–Oppenheimer qui consistent en la contrainte homogène ainsi qu'en une énergie supplémentaire provenant des bandes d'énergie des perturbations de Fock. Les réactions inverses des gravitons ne jouent aucun rôle à cet ordre et ils ne restent que les contributions du champ de Mukhanov–Sasaki. Celles-ci incluent les masses indéfinies effectives qui conduiraient donc à des divergences de la fonction symbolique. De plus, la contrainte dépend de manière non–triviale des variables de l'espace des phases homogène, ce qui complique considérablement la recherche d'un domaine de la contrainte et des solutions possibles.

Par conséquent, nous discutons plusieurs stratégies pour surmonter les problèmes liés aux masses carrées indéfinies et aux instabilités tachyoniques correspondantes. La première proposition consiste à examiner les transformations possibles qui ont effectivement conduit aux instabilités tachyoniques. Une deuxième proposition consiste à restreindre l'espace des phases homogène d'une manière appropriée afin que les masses au carré deviennent manifestement positives. Ceci peut être réalisé en trouvant une transformation canonique appropriée dans le secteur homogène. Une telle stratégie a été employée pour le modèle inhomogène avec champ de poussière, et nous avons également discuté une modification similaire du modèle avec perturbations cosmologiques invariantes de jauge. La contrainte hamiltonienne effective qui en résulte contient également les effets des réactions inverses des modes tensoriels. Une telle transformation peut restreindre l'espace des phases original au sens que les nouvelles variables ne sont définies que sur des intervalles compacts de l'espace des phases original. Par conséquent, la procédure de quantification de Weyl et le produit étoile doivent être soigneusement révisée. De plus, la contrainte effective dépend toujours de manière non–triviale et non–polynomiale des degrés de liberté homogènes, ce qui rend la recherche d'un domaine de définition et de solutions possibles difficile. Nous reportons cette question à des recherches futures.

Pour conclure, nous soulignons que la théorie des perturbations spatio–adiabatique s'applique en principe à tout modèle qui admet un paramètre perturbatif approprié, résultant des rapports des masses ou des constantes de couplage de deux sous–systèmes. Dans le cas d'un vrai hamiltonien physique, le système doit en outre éviter les puissances inverses du paramètre perturbatif. Pour un système contraint, il est par contre toujours possible de multiplier la contrainte par des facteurs appropriés du paramètre perturbatif pour éviter des telles puissances inverses. Cependant, le raisonnement usuel selon lequel le système associé avec une masse lourde évolue à une vitesse inférieure à celle du système léger, ne s'applique pas au cas contraint.

IV.11. Perspectives d'Avenir

Malgré des nombreux résultats et conclusions obtenus au cours de cette thèse, l'application de la théorie des perturbations spatio–adiabatiques aux systèmes cosmologiques pose également certaines questions importantes et propose plusieurs nouvelles directions de recherche.

Une extension évidente de nos résultats serait de poursuivre le schéma perturbatif jusqu'à des ordres plus élevés. Nous nous sommes limités au second ordre, mais la construction de ré-

sultats à des ordres supérieurs bien que possible, pourrait être laborieuse. Nous avons énoncé les bases d'une telle entreprise en effectuant une construction itérative du schéma perturbatif pour chaque ordre possible.

Vis–à–vis des contraintes effectives résultantes du schéma, nous soulignons aussi qu'elles dépendent de manière non–polynomiale des variables de l'espace des phases lentes ou homogènes dans tous les cas considérés ici. On peut s'attendre à ce que le degré de non polynomialité augmente avec l'ordre du schéma considéré car les coefficients de connexion non–polynomiaux contribuent à des ordres proportionnellement plus élevés. Par conséquent, pour certaines régions de l'espace des phases, l'hamiltonien admet un comportement singulier. Étant donné que l'objectif principal du schéma est de procéder avec une quantification de Weyl des hamiltoniens effectifs par rapport au secteur lent ou homogène, la non–polynomialité pourrait affecter sérieusement la recherche d'un domaine ou de solutions invariants de l'opérateur. Nous avons souligné qu'un domaine invariant peut être trouvé pour un type spécifique de fonctions symboliques.

Une autre difficulté liée à ce problème précédent concerne les carrés des masses indéfinis pour les modèles inhomogènes. Une solution évidente pour cela serait de réviser les transformations pour le système entier qui ont généré ces fonctions de masse effectives. Même si nous avons commençé par considérer des transformations génériques au début, nous avons restreint nos considérations à une transformation spécifique dans les applications suivantes. Une autre stratégie est d'aborder des transformations ou des plongements canoniques par rapport à l'espace des phases homogène afin d'obtenir des fonctions de masse au carré positif. En effet, nous avons employé cette stratégie pour deux modèles inhomogènes. Pour le modèle avec des perturbations invariantes de jauge, ce plongement aboutit à la restriction d'une des variables à une union de deux intervalles compactes. En conséquence, il faut réviser les règles et la procédure de la quantification de Weyl attentivement.

Enfin, l'une des questions les plus importantes en cosmologie concerne la comparaison de nos résultats avec des données expérimentales. L'approche naturelle qui prendrait en compte les effets quantiques de notre approche fonctionne comme suit: Partant de la contrainte effective du modèle inhomogènes aux variables invariantes de jauge, on détermine les solutions de cette contrainte, c'est–à–dire qu'on essaie de trouver des états dans l'espace de Hilbert qui sont annihilés par la contrainte quantique. Puis, on applique la quantification de Weyl du symbole unitaire qu'on a construit auparavant. Cela donnera un état dans l'espace de Hilbert total et qui correspond à des vraies solutions à une erreur d'ordre trois dans le paramètre adiabatique. Idéalement, cet état suit une trajectoire semi–classique au moins par rapport aux variables homogènes. On pourrait alors extraire des trajectoires relationnelles du champs scalaire et du facteur d'échelle (cela pourrait générer un paramètre de temps interne). Finalement, on pourrait évaluer les spectres de puissances des modes inhomogènes au long de cette trajectoire. Les amplitudes des modes donneraient un spectre de puissance primordial.

Sachant que trouver ces solutions est très difficile (même impossible), on pourrait suivre un chemin plus modeste inspiré par le théorème d'Egorov. Il est basé sur l'idée que l'évolution temporelle d'une observable semi–classique en mécanique quantique suit, à des erreurs près, la trajectoire classique et a des propriétés "semi–classiques". Par conséquent, son évolution peut être obtenue par un transport le long du flux classique générés par l'hamiltonien classique. De manière similaire, on peut transporter les champs quantiques inhomogènes le long du flux généré

par l'hamiltonien effectif.

Finalement, nous soulignons également que nous avons toujours considéré des théories linéaires dans les perturbations cosmologiques. Il s'agit bien entendu d'une approximation qui n'est plus valable dès que l'amplitude des modes devient trop grande. Une extension possible serait donc de considérer des théorie des perturbations cosmologiques d'ordre supérieur.

Part V.

Appendix

A. Computation for the Born–Oppenheimer Approximation

In this section, we give some of the calculations underlying the results of section 6.1, and which we think are beneficial for the understanding of the results, in particular because these calculations are not given in the original references by Chruściński and Jamiołkowksi (2004), Panati, Spohn, and Teufel (2007), and Stottmeister and Thiemann (2016a).

As introduced in section 6.1, we use the generalized basis states $\{T_{(q_0,n)}\}$ of the electronic Hamilton operator $H_\mathrm{f}(\hat{q};\boldsymbol{x},\boldsymbol{y})$ which are distributions on $\mathcal{S}(\mathbb{R}^N)\otimes\mathcal{H}_\mathrm{f}\subset L^2(\mathbb{R}^N)\otimes\mathcal{H}_\mathrm{f}$ labelled by $q_0\in\mathbb{R}$ and $n\in\mathbb{N}$. For some $\psi(q)\in\mathcal{S}(\mathbb{R}^N)$ and $\phi\in\mathcal{S}(\mathbb{R}^K)\subset\mathcal{H}_\mathrm{f}$, they are defined to yield $T_{(q_0,n)}(\psi\otimes\phi)=\psi(q_0)\otimes\langle\phi_n(q_0),\phi\rangle_{\mathcal{H}_\mathrm{f}}$. Recall that the $\{T_{(q_0,n)}\}$ build indeed a complete generalized eigenbasis of $L^2(\mathbb{R}^N)\otimes\mathcal{H}_\mathrm{f}\cong L^2(\mathbb{R}^N,\mathcal{H}_\mathrm{f})$ if we assume that $H_\mathrm{f}(\hat{q};\boldsymbol{x},\boldsymbol{y})$ is essentially self–adjoint on $\mathcal{S}(\mathbb{R}^N)\otimes\mathcal{S}(\mathbb{R}^K)$ (Gel'fand and N. Y. Vilenkin 1964, p. 120). Often, it is intuitive to use a formal integral notation regarding the first tensor factor using delta distributions

$$T_{(q_0,n)}=\int_{\mathbb{R}}\mathrm{d}q\,\delta(q-q_0)\otimes\langle\phi_n(q_0),\cdot\,\rangle_{\mathcal{H}_\mathrm{f}}. \tag{A.1}$$

We can picture elements in $\mathcal{S}(\mathbb{R}^N,\mathcal{H}_\mathrm{f})$ as Schwartz functions over $\mathbb{R}^N$ which accomodate some vector $\phi\in\mathcal{H}_\mathrm{f}$ at every point $q\in\mathbb{R}^N$. This corresponds to a fibre bundle over $\mathbb{R}^N$ with fibres $\mathcal{H}_\mathrm{f}=\mathcal{H}_\mathrm{f}(q)$ at every point $q\in\mathbb{R}^N$. It is therefore reasonable to consider vector fields $\phi(q)\in C^\infty(\mathbb{R}^N,\mathcal{H}_\mathrm{f})$ such that for every $q\in\mathbb{R}^N$ it is $\phi(q)\in\mathcal{H}_\mathrm{f}$. Such a vector field is obtained by regarding $H_\mathrm{f}(q;\boldsymbol{x},\boldsymbol{y})$ as a q–dependent operator on $\mathcal{H}_\mathrm{f}$ and determining its eigensolutions $\{\phi_n(q)\}_{n\in\mathbb{N}^K}$ for every $q\in\mathbb{R}^N$, namely

$$H_\mathrm{f}(q;\boldsymbol{x},\boldsymbol{y})\phi_n(q)=\epsilon_n(q)\phi_n(q),\quad\forall q\in\mathbb{R}^N,\ \forall n\in\mathbb{N}^K. \tag{A.2}$$

For some fixed $q_0\in\mathbb{R}^N$, the states $\{\phi_n(q_0)\}_{n\in\mathbb{N}^K}$ represent a certain basis choice in $\mathcal{H}_\mathrm{f}$. The distributions $T_{(q_0,n)}$ simply project on the value of the wave function at q_0 and the associated basis state $\phi_n(q_0)\in\mathcal{H}_\mathrm{f}$ at this point.

As suggested in section 6.1, we consider the solution $\Psi^E\in\mathcal{H}$ of the total Hamiltonian $\hat{\boldsymbol{H}}$ which satisfies

$$\hat{\boldsymbol{H}}\,\Psi^E=E\,\Psi^E. \tag{A.3}$$

We can write its projection to some point q_0 and the vector $\phi_n(q_0)$ by means of $T_{(q_0,n)}$ such that

$$\begin{aligned} E\psi_n^E(q_0) &:= E\,T_{(q_0,n)}(\Psi^E) = E\int_{\mathbb{R}^N} \mathrm{d}q\,\delta(q-q_0)\langle\phi_n(q_0),\cdot\,\rangle_{\mathcal{H}_\mathrm{f}}\,\Psi^E(q) \\ &= \int_{\mathbb{R}^N} \mathrm{d}q\,\delta(q-q_0)\langle\phi_n(q_0),\cdot\,\rangle_{\mathcal{H}_\mathrm{f}}\,\widehat{\boldsymbol{H}}\Psi^E(q) \\ &= \int_{\mathbb{R}^N} \mathrm{d}q\,\delta(q-q_0)\langle\phi_n(q_0),\cdot\,\rangle_{\mathcal{H}_\mathrm{f}}\left(\frac{\varepsilon^2}{m}(-i\nabla_q + A(q))^2 + H_\mathrm{f}(\hat{q};\boldsymbol{x},\boldsymbol{y})\right)\Psi^E(q) \end{aligned} \tag{A.4}$$

To solve the second electronic contribution in the last line, we use the position–Schrödinger representation of the electronic Hamiltonian with respect to the nucleonic degrees of freedom, i.e., the operator acts as a multiplication operator with regard to q. Furthermore, let us implement a unity operator using the *complete* generalized basis $T_{(q',n')}$, in particular

$$(\hat{\mathbf{1}}_{\mathcal{H}}\Psi^E)(q) = \sum_{n'}\int_{\mathbb{R}^N} \mathrm{d}q'\,T_{(q',n')}(q)\,T_{(q',n')}(\Psi^E) \tag{A.5}$$

$$= \sum_{n'}\int_{\mathbb{R}^N} \mathrm{d}q'\,\delta(q'-q)\,\phi_{n'}(q)\,\psi_{n'}^E(q') = \sum_{n'}\phi_{n'}(q)\psi_{n'}^E(q). \tag{A.6}$$

The second, electronic term in the previous equation (A.4) consequently yields

$$\begin{aligned} &\int_{\mathbb{R}^N} \mathrm{d}q\,\delta(q-q_0)\,\langle\phi_n(q_0),\cdot\,\rangle_{\mathcal{H}_\mathrm{f}}\,H_\mathrm{f}(q;\boldsymbol{x},\boldsymbol{y})(\hat{\mathbf{1}}_{\mathcal{H}}\Psi^E)(q) \\ &= \int_{\mathbb{R}^N} \mathrm{d}q\,\delta(q-q_0)\,\langle\phi_n(q_0),\cdot\,\rangle_{\mathcal{H}_\mathrm{f}}\sum_{n'} H_\mathrm{f}(q;\boldsymbol{x},\boldsymbol{y})\,\phi_{n'}(q)\,\psi_{n'}^E(q) \\ &= \int_{\mathbb{R}^N} \mathrm{d}q\,\delta(q-q_0)\,\langle\phi_n(q_0),\cdot\,\rangle_{\mathcal{H}_\mathrm{f}}\sum_{n'} E_{\mathrm{f},n'}(q)\phi_{n'}(q)\,\psi_{n'}^E(q) = E_{\mathrm{f},n}(q_0)\,\psi_{n'}^E(q_0) \end{aligned} \tag{A.7}$$

because $\sum_{n'}\langle\phi_n(q_0),\phi_{n'}(q_0)\rangle_{\mathcal{H}_\mathrm{f}} = 1$. To compute the kinetic term in (A.4), it is useful to first apply only one factor $(-i\nabla_q + A(q))$ to $\Psi^E(q)$ which yields using the product rule of derivations

$$\begin{aligned} (-i\nabla_q + A(q))(\hat{\mathbf{1}}_{\mathcal{H}}\Psi^E)(q) &= (-i\nabla_q + A(q))\sum_{n'}\phi_{n'}(q)\,\psi_{n'}^E(q) \\ &= \sum_{n'}(-i\nabla_q\phi_{n'})(q)\,\psi_{n'}^E(q) + \phi_{n'}(q)\left((-i\nabla_q + A(q))\psi_{n'}^E\right)(q). \end{aligned} \tag{A.8}$$

To obtain the final matrix element, we employ also the second factor $(-i\nabla_q + A(q))$ and eventually apply the distribution $T_{(q_0,n)}$. To begin with, let us consider only the first term of the above interim

result. Using the product rule for derivations (after the second equality sign), we obtain

$$
\begin{aligned}
&\int_{\mathbb{R}^N} \mathrm{d}q\, \delta(q-q_0)\, \langle \phi_n(q_0), \cdot \rangle_{\mathcal{H}_\mathrm{f}} (-i\nabla_q + A(q)) \sum_{n'} (-i\nabla_q \phi_{n'})(q)\, \psi^E_{n'}(q) \qquad \text{(A.9)}\\
&= \langle \phi_n(q_0), \cdot \rangle_{\mathcal{H}_\mathrm{f}} (-i\nabla_{q_0} + A(q_0)) \sum_{n'} (-i\nabla_{q_0} \phi_{n'})(q_0)\, \psi^E_{n'}(q_0)\\
&= (-i\nabla_{q_0} + A(q_0)) \sum_{n'} \langle \phi_n(q_0), (-i\nabla_{q_0}\phi_{n'}(q_0)) \rangle_{\mathcal{H}_\mathrm{f}}\, \psi^E_{n'}(q_0)\\
&\quad + \sum_{n'} \langle ((-i\nabla_{q_0}\phi_n)(q_0), \cdot \rangle_{\mathcal{H}_\mathrm{f}} (-i\nabla_{q_0}\phi_{n'})(q_0)\, \psi^E_{n'}(q_0)\\
&= -(\nabla_{q_0} + iA(q_0)) \sum_{n'} \langle \phi_n(q_0), (\nabla_{q_0}\phi_{n'})(q_0) \rangle_{\mathcal{H}_\mathrm{f}}\, \psi^E_{n'}(q_0)\\
&\quad + \sum_{n'} \langle ((-i\nabla_{q_0}\phi_n)(q_0), \cdot \rangle_{\mathcal{H}_\mathrm{f}} \sum_{n''} \phi_{n''}(q_0) \langle \phi_{n''}(q_0), \cdot \rangle_{\mathcal{H}_\mathrm{f}} (-i\nabla_{q_0}\phi_{n'})(q_0)\, \psi^E_{n'}(q_0)\\
&= -(\nabla_{q_0} + iA(q_0)) \sum_{n'} \langle \phi_n(q_0), (\nabla_{q_0}\phi_{n'})(q_0) \rangle_{\mathcal{H}_\mathrm{f}}\, \psi^E_{n'}(q_0)\\
&\quad - \sum_{n',n''} \langle \phi_n(q_0), (\nabla_{q_0}\phi_{n'})(q_0) \rangle_{\mathcal{H}_\mathrm{f}} \langle \phi_{n'}(q_0), (\nabla_{q_0}\phi_{n''})(q_0) \rangle_{\mathcal{H}_\mathrm{f}}\, \psi^E_{n''}(q_0)
\end{aligned}
$$

where we inserted a unity operator $\mathbf{1}_{\mathcal{H}_\mathrm{f}}$ in the last step. Analogously, we apply $(-i\nabla_q + A(q))$ and $T_{(q_0,n)}$ to the two latter contributions in equation (A.8) which gives

$$
\begin{aligned}
&\int_{\mathbb{R}^N} \mathrm{d}q\, \delta(q-q_0)\, \langle \phi_n(q_0), \cdot \rangle_{\mathcal{H}_\mathrm{f}} \left(-i\nabla_q + A(q)\right) \sum_{n'} \phi_{n'}(q) \left(\left(-i\nabla_q + A(q)\right) \psi^E_{n'} \right)(q)\\
&= -\sum_{n'} \langle \phi_n(q_0), \left(\nabla_{q_0}\phi_{n'}\right)(q_0) \rangle_{\mathcal{H}_\mathrm{f}} \left((\nabla_{q_0} + iA(q_0))\psi^E_n \right)(q_0) - \left((\nabla_{q_0} + iA(q_0))^2 \psi^E_n \right)(q_0). \qquad \text{(A.10)}
\end{aligned}
$$

To condense the previous computations, it is convenient to introduce the matrix elements (Stottmeister and Thiemann 2016a)

$$
\begin{aligned}
\mathcal{A}_n^{\ n'}(q_0) &:= -i \langle \phi_n(q_0), (\nabla_{q_0}\phi_{n'})(q_0) \rangle_{\mathcal{H}_\mathrm{f}}, \qquad \text{(A.11)}\\
D_n^{\ n'}(q_0) &:= \delta_n^{\ n'} \left(\nabla_{q_0} + iA(q_0) \right) - i\mathcal{A}_n^{\ n'}(q_0). \qquad \text{(A.12)}
\end{aligned}
$$

The final outcome for the matrix element $E\,\psi^E_n(q_0)$ in equation (A.4) emanates from the interim results (A.7), (A.9) and (A.10), together with the definitions (A.11) and (A.12), and is given by

$$
E\,\psi^E_n(q_0) = \sum_{n''} \left(-\frac{\varepsilon^2}{m} \sum_{n'} D_n^{\ n'}(q_0)\, D_{n'}^{\ n''}(q_0) + \epsilon_n(q_0)\, \delta_n^{\ n''} \right) \psi^E_{n''}(q_0). \qquad \text{(A.13)}
$$

B. Oscillator Effective Solutions

In this section, we detail the application of standard quantum mechanical perturbation theory to the oscillator model of section 6.8. Our considerations are based and largely taken from (Neuser, Schander, and Thiemann 2019).

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

$$h^{\text{kin}}_{\text{eff},2,\text{R}}(q,p) := -\frac{L^2\left(\nu+\frac{1}{2}\right)}{2M^2\Omega_0}\cdot\frac{p^2q^2}{(L^2+q^2)^3}, \tag{B.1}$$

$$h^{\text{pot}}_{\text{eff},2,\text{R}}(q) := \frac{\nu^2+\nu+1}{4M}\cdot\frac{q^2}{(L^2+q^2)^2}. \tag{B.2}$$

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

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

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

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

$$H_d(u_\nu) = d! \sum_{m=0}^{\lfloor \frac{d}{2} \rfloor} \frac{(-1)^m}{m!(d-2m)!} (2u_\nu)^{d-2m} \tag{B.4}$$

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

$$I(\lambda) := \int_{\mathbb{R}} e^{-u_\nu^2} \frac{u_\nu^{2\lambda}}{(\ell_\nu^2 + u_\nu^2)^2} \, \mathrm{d}u_\nu, \quad J(\lambda) := \int_{\mathbb{R}} e^{-u_\nu^2} \frac{u_\nu^{2\lambda}}{(\ell_\nu^2 + u_\nu^2)^3} \, \mathrm{d}u_\nu \tag{B.5}$$

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

$$I(\lambda) = \Gamma\left(\lambda - \frac{3}{2}\right) - 2\ell_\nu^2 I(\lambda - 1) - \ell_\nu^4 I(\lambda - 2) \tag{B.6}$$

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

$$I(\lambda) := a(\lambda) I(0) + b(\lambda) I(1) + \sum_{i=2}^{\lambda} c_i(\lambda) \, \Gamma\left(i - \frac{3}{2}\right). \tag{B.7}$$

in equation (B.6) and we determine the coefficients to be

$$a(\lambda) = (1-\lambda)(-1)^\lambda \ell_\nu^{2\lambda}, \tag{B.8}$$

$$b(\lambda) = \lambda(-1)^{\lambda-1} \ell_\nu^{2(\lambda-1)}, \tag{B.9}$$

$$c_i(\lambda) = (1+\lambda-i)(-1)^{\lambda-i} \ell_\nu^{2(\lambda-i)}. \tag{B.10}$$

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

$$\Delta E_{d,\nu}^{\mathrm{pot}} = \frac{\Omega_\nu 2^d d! (\nu^2 + \nu + 1)}{4\hbar\sqrt{\pi}} \sum_{m=0}^{\lfloor \frac{d}{2} \rfloor} \sum_{k=0}^{\lfloor \frac{d}{2} \rfloor} \frac{(-1)^{m+k} 2^{-2(m+k)}}{m!k!(d-2m)!(d-2k)!} I(d-m-k+1) \tag{B.11}$$

and likewise for the kinetic term but more lengthy. By evaluating the sums and employing the specific $I(\lambda)$'s for every summand, we obtain the correct energy shift. Namely, the energy shifts

for $d = 0$ and $d = 1$ are given by

$$\Delta E_{0,\nu} = \frac{\Omega_\nu(\nu^2+\nu+1)}{4\sqrt{\pi}} I(1) + \frac{\ell_\nu^2 \Omega_\nu^2 \left(\nu+\frac{1}{2}\right)}{4\sqrt{\pi}\Omega_0}(2J(1)-J(2)), \tag{B.12}$$

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

with the integrals given by

$$I(0) = \frac{\sqrt{\pi}}{\ell_\nu^2} + \frac{\pi}{2\ell_\nu^3} e^{\ell_\nu^2}(2\ell_\nu^2-1)(\mathrm{erf}(\ell_\nu)-1), \tag{B.13}$$

$$I(1) = -\sqrt{\pi} - \frac{\pi}{2\ell_\nu} e^{\ell_\nu^2}(1+2\ell_\nu^2)(\mathrm{erf}(\ell_\nu)-1), \tag{B.14}$$

$$J(1) = \frac{\sqrt{\pi}}{4\ell_\nu^2}(1+2\ell_\nu^2) + \frac{\pi}{8\ell_\nu^3} e^{\ell_\nu^2}\left(1-4\ell_\nu^2-4\ell_\nu^4\right)(1-\mathrm{erf}(\ell_\nu)), \tag{B.15}$$

$$J(2) = -\frac{\sqrt{\pi}}{4}(5+2\ell_\nu^2) + \frac{\pi}{8\ell_\nu} e^{\ell_\nu^2}\left(3+12\ell_\nu^2+4\ell_\nu^4\right)(1-\mathrm{erf}(\ell_\nu)). \tag{B.16}$$

Here, “erf” denotes the error function. Employing the integrals in the above equations yields the expressions in equation (6.221).

C. Weyl Quantization on a Compact Interval

In this section, we elaborate on the Weyl quantization procedure for a system whose configuration space is restricted to a compact interval. Without loss of generality, let us consider $x \in I := [0, 2\pi]$. We start by stating our conventions for the Fourier transform and the Fourier series.

In the case that $x \in \mathbb{R}$ and $f \in \mathcal{S}(\mathbb{R})$, we choose the Fourier transform of f to have the form

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \check{f}(\xi)\, e^{i\xi x} \mathrm{d}\xi, \qquad \check{f}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(x)\, e^{-i\xi x} \mathrm{d}x \tag{C.1}$$

where $\check{f} \in \mathcal{S}(\mathbb{R})$ is the Fourier transform of f.

In contrast, let $x \in I$ and $f \in L^2(I)$. The Fourier series of f is given by

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \check{f}_n\, e^{inx}, \qquad \check{f}_n = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} f(x)\, e^{-inx} \mathrm{d}x \tag{C.2}$$

where $\check{f}_n \in l^2(\mathbb{Z})$ are the Fourier mode coefficients.

Now, let $A : I \times \mathbb{R} \to \mathbb{R}$ be a real–valued function on the phase space $I \times \mathbb{R}$. Its Weyl quantization is defined by its Fourier transform (with respect to both variables) $\check{A}$ using Weyl elements by

$$A(\hat{x}, \hat{p}) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \int_{\mathbb{R}} \mathrm{d}\xi \check{A}(n, \xi)\, e^{in\hat{x} + i\xi\hat{p}}. \tag{C.3}$$

In order to know the action of the Weyl elements on a wave function, one must choose one particular self–adjoint extension of the momentum operator $\hat{p}$ on the interval I. In fact, there is an infinite number of extensions and which can be parametrized by a complex number α. This number defines how the wave function at $x = 2\pi$ is related to the wave function at $x = 0$, i.e., $\psi(0) = \alpha\psi(2\pi)$, see (Reed and Simon 1975b) for details. Let us consider the case $\alpha = 1$ here. Then, for a wave function $\psi \in C_0^\infty(I)$ with $\psi(0) = \psi(2\pi)$, the Weyl element acts as

$$(e^{in\hat{x} + i\xi\hat{p}}\psi)(x) = e^{\frac{1}{2}in\xi} e^{inx} \psi(x + \xi \mod 2\pi). \tag{C.4}$$

Employing this relation into equation (C.3) when applied to a suitable wave function yields (after

the first line we omit the $\mod 2\pi$ for notational reasons)

$$(A(\hat{x},\hat{p})\psi)(x) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\int_{\mathbb{R}} \mathrm{d}\xi \check{A}(n,\xi)\, e^{\frac{i}{2}n\xi+inx}\psi(x+\xi \mod 2\pi) \tag{C.5}$$

$$= \frac{1}{4\pi^2}\sum_{n=-\infty}^{\infty}\int_{\mathbb{R}} \mathrm{d}\xi \left(\int_0^{2\pi}\mathrm{d}y\int_{\mathbb{R}}\mathrm{d}p\, A(y,p)\, e^{-iny-i\xi p}\right) e^{\frac{i}{2}n\xi+inx}\psi(x+\xi) \tag{C.6}$$

$$= \frac{1}{4\pi^2}\int_{\mathbb{R}}\mathrm{d}\xi\int_0^{2\pi}\mathrm{d}y\int_{\mathbb{R}}\mathrm{d}p\, A(y,p)\left(\sum_{n=-\infty}^{\infty} e^{-iny+inx+\frac{i}{2}n\xi}\right)e^{-i\xi p}\psi(x+\xi)$$

$$= \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\xi\int_0^{2\pi}\mathrm{d}y\int_{\mathbb{R}}\mathrm{d}p\, A(y,p)\left(\sum_{k=-\infty}^{\infty}\delta\left(y-x-\frac{1}{2}\xi+2\pi k\right)\right)e^{-i\xi p}\psi(x+\xi)$$

where we employed the definition of the Dirac comb in order to get the last equality. We then define a new variable $z := y - x - \frac{1}{2}\xi$. Besides, we define a function $k(x,\xi)$ that selects the one particular k such that the integral does not vanish for a fixed configuration (x,ξ), i.e.,

$$(A(\hat{x},\hat{p})\psi)(x) = \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\xi\int_{\mathbb{R}}\mathrm{d}p\int_{-x-\frac{1}{2}\xi}^{2\pi-x-\frac{1}{2}\xi}\mathrm{d}z A\left(z+x+\frac{1}{2}\xi,p\right)\delta(z+2\pi k(x,\xi))e^{-i\xi p}\psi(x+\xi)$$

$$= \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\xi\int_{\mathbb{R}}\mathrm{d}p\, A\left(x+\frac{1}{2}\xi-2\pi k(x,\xi),p\right)e^{-i\xi p}\psi(x+\xi) \tag{C.7}$$

$$= \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\xi\int_{\mathbb{R}}\mathrm{d}p\, A\left(x+\frac{1}{2}\xi \mod 2\pi,p\right)e^{-i\xi p}\psi(x+\xi \mod 2\pi). \tag{C.8}$$

We split the integral over ξ into an infinite number of integrals of length $[0,2\pi]$, and for the second equality we define a new variable $\xi' := \xi - 4\pi n$ such that

$$(A(\hat{x},\hat{p})\psi)(x) = \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}p\sum_{n=-\infty}^{\infty}\int_{4\pi n-2x}^{4\pi(n+1)-2x}\mathrm{d}\xi\, A\left(x+\frac{1}{2}\xi \mod 2\pi,p\right)e^{-i\xi p}\psi(x+\xi \mod 2\pi)$$

$$= \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}p\sum_{n=-\infty}^{\infty}\int_{-2x}^{4\pi-2x}\mathrm{d}\xi' A\left(x+\frac{1}{2}\xi' \mod 2\pi,p\right)e^{-i(\xi'+4\pi n)p}\psi(x+\xi' \bmod 2\pi).$$

Then, we interchange the integral over ξ' and the sum and use again the definition of the Dirac comb which gives

$$(A(\hat{x},\hat{p})\psi)(x) = \int_{\mathbb{R}}\mathrm{d}p\int_{-2x}^{4\pi-2x}\mathrm{d}\xi' A\left(x+\frac{1}{2}\xi' \mod 2\pi,p\right)e^{-i\xi' p}\psi(x+\xi' \mod 2\pi) \tag{C.9}$$

$$\cdot\sum_{k=-\infty}^{\infty}\frac{1}{4\pi}\delta\left(p-\frac{k}{2}\right)$$

$$= \sum_{k=-\infty}^{\infty}\int_{-2x}^{4\pi-2x}\mathrm{d}\xi'\frac{1}{4\pi}A\left(x+\frac{1}{2}\xi' \mod 2\pi,\frac{k}{2}\right)e^{-i\xi'\frac{k}{2}}\psi(x+\xi' \mod 2\pi).$$

(C.10)

Finally, we define $y := \xi' + x$ in order to replace ξ' and obtain

$$(A(\hat{x}, \hat{p})\psi)(x) = \frac{1}{4\pi} \sum_{k=-\infty}^{\infty} \int_{-x}^{4\pi-x} \mathrm{d}y A\left(\frac{1}{2}(x+y), \frac{k}{2}\right) e^{-i\frac{k}{2}(y-x)} \psi(y \mod 2\pi). \tag{C.11}$$

One can easily check that this definition for the Weyl quantization leads exactly the standard Weyl prescriptions. For $A(x) = e^{i\lambda x}$ and $x \in (0, 2\pi)$, we get

$$(A(\hat{x})\psi)(x) = e^{i\lambda x}\psi(x). \tag{C.12}$$

For $A(p) = e^{i\lambda p}$, and $x \in (0, 2\pi)$, we have

$$(A(\hat{p})\psi)(x) = \psi(x + \lambda \mod 2\pi). \tag{C.13}$$

Let $A(p) = p$, $x \in (0, 2\pi)$. Then, we get

$$(A(\hat{p})\psi)(x) = -i\frac{\partial\psi(x)}{\partial x}. \tag{C.14}$$

List of Symbols and Acronyms

$\mathcal{A}_Q$	Quantum field Weyl algebra
$\mathcal{B}$	Space of bounded operators on some Hilbert space
$\mathcal{F}_s$	Symmetric Fock space on some one–particle Hilbert space
$\mathbb{k}$	Space of discrete mode vectors on the three–torus, excluding zero, i.e., $\mathbb{k} := 2\pi\mathbb{Z}^3 \setminus \{0\}$
$\mathbb{K}$	Space of discrete mode vectors on the three–torus, excluding zero, and a label $\tau = \pm$ distinguishing two tensor modes, i.e., $\mathbb{K} := (2\pi\mathbb{Z}^3 \setminus \{0\}, \pm)$
κ	Inverse of the reduced Planck mass squared, $\kappa = 8\pi G = M_{\mathrm{Pl}}^{-2}$
$\mathcal{L}$	Space of linear operators on some Hilbert space
λ	A generic matter coupling constant
Λ	Cosmological constant
$\tilde{\Lambda}$	Rescaled cosmological constant, $\tilde{\Lambda} := \frac{\Lambda}{\epsilon^2}$
$\mathcal{M}$	Space time manifold, four–dimensional
M_{Pl}	Reduced Planck mass $M_{\mathrm{Pl}} = \sqrt{\hbar c/(8\pi G)}$
G	Newton's constant
T	Bundle of (r, s)–tensors over some manifold
$\mathbb{T}^3$	The three–torus $\mathbb{T}^3 = S^1 \times S^1 \times S^1$
z	Cosmological redshift
ADM	Arnowitt–Deser–Misner formalism for performing a $(3+1)$–split of a four–dimensional spacetime
CDM	Cold dark matter
CMB	Cosmic microwave background, see section 2.2
CTP CGEA	Closed time path coarse grained effective action
FLRW	Friedmann–Lemaître–Robertson–Walker solutions of the metric tensor, see section 2.2.1
GNS	Gel'fand–Naimark–Segal construction of QFT on CST
ΛCDM	Lambda cold dark matter model of the Universe, see section 2.2
LQC	Loop quantum cosmology
LQG	Loop quantum gravity
QFT	Quantum field theory
QFT on CST	Quantum field theory on curved space times
SAPT	Space adiabatic perturbation theory

WKB	Wentzel–Kramers–Brillouin (semiclassical) approximation

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